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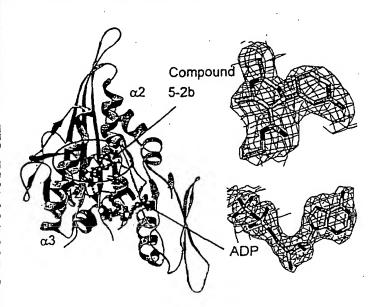
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[Continued on next page]

(54) Title: MITOTIC KINESIN BINDING SITE



(57) Abstract: The present invention is directed to the identification, characterization and three-dimensional structure of a novel ligand binding site of KSP. Binding of ligands to the novel binding site result in a conformational change in the three-dimensional structure of the protein and a modulation of the activity of KSP. This conformational change in turn results in the formation of a novel binding pocket in the KSP protein, which comprises the novel binding site of the instant invention.

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TITLE OF THE INVENTION MITOTIC KINESIN BINDING SITE

FIELD OF THE INVENTION

5 The present invention generally pertains to the fields of molecular biology, protein purification, protein crystallization, X-ray diffraction analysis, three-dimensional structural determination, rational drug design and molecular modeling of motor proteins, in particular -Kinesin Spindle Protein (KSP). Compositions and crystals of KSP with a 10 KSP inhibitor bound to the protein at the novel ligand binding site identified herein are also provided. The crystallized KSP is physically analyzed by Xray diffraction techniques. The resulting X-ray diffraction patterns are of sufficiently high resolution to be useful for determining the threedimensional structure of inhibitor-bound KSP. Those atomic coordinates are useful in molecular modeling of related proteins and rational drug design 15 (RDD) of mimetics and ligands for KSP and related proteins. Methods of using the structure coordinates of KSP in complex with an inhibitor for the design of pharmaceutical compositions which inhibit the biological function of KSP, particularly those biological functions mediated by molecular interactions involving KSP are also disclosed. 20

BACKGROUND OF THE INVENTION

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Cancer remains one of the leading causes of death in the United States. Clinically, a broad variety of medical approaches, including surgery, radiation therapy and chemotherapeutic drug therapy are currently being used in the treatment of human cancer (see the textbook CANCER: Principles & Practice of Oncology, 6th Edition, De Vita et al., eds., J. B. Lippincott Company, Philadelphia, Pa., 2001). However, it is recognized that such approaches continue to be limited by a fundamental lack of a clear understanding of the precise cellular bases of malignant transformation and neoplastic growth.

The control of cell division is one of the most basic aspects of multicellular existence. Uncontrolled cell growth and division, which produces cells that divide when they should not, produces contiguous cellular masses called tumors that are the basis for many cancers.

A common strategy for cancer therapy is the development of drugs that interrupt the cell cycle during mitosis. Compounds that perturb shortening (depolymerization) or lengthening (polymerization) cause arrest of the cell cycle in mitosis due to perturbation of the normal microtubule dynamics necessary for the chromosome movement. (Compton, D. A., et al., (1999) Science 286:913-914). A common denominator attending these compounds is that they arrest cells in mitosis by inhibiting spindle assembly (Compton, D. A., et al., (1999) Science 286:313-314). More recently, some agents such as monastrol have been implicated in inhibiting mitosis by blocking the function of essential proteins, such as mitotic proteins. (Mayer, T.U. et al., (1999) Science 286: 971-974).

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The motor protein, kinesin, was discovered in 1985 in squid axoplasm. R. D. Vale et al., Identification of a Novel Force-generating Protein, Kinesin, Involved in Microtubule-based Motility, *Cell* 42:39-50 (1985). In the last few years, it has been discovered that kinesin is just one member of a very large family of motor proteins. E.g., S. A. Endow, The Emerging Kinesin Family of Microtubule Motor Proteins, 16 Trends Biochem. Sci. 221 (1991); L. S. B. Goldstein, The Kinesin Superfamily: Tails of Functional Redundancy, 1 Trends Cell Biol. 93 (1991); R. J. Stewart et al., Identification and Partial Characterization of Six Members of

Stewart et al., Identification and Partial Characterization of Six Members of the Kinesin Superfamily in Drosophila. Proc. Nat'l Acad. Sci. USA 88:8470 (1991). Other motor proteins include dynein, e.g. M.-G. Li et al., Drosophila Cytoplasmic Dynein, a Microtubule Motor that is Asymmetrically Localized in the Oocyte, J. Cell Biol. 126:1475-1493 (1994), and myosin, e.g. T. Q. P.
 Uyeda et al., J. Mol. Biol. 214:699-710 (1990).

Mitotic kinesins are enzymes essential for assembly and function of the mitotic spindle, but are not generally part of other microtubule structures, such as in nerve processes. These essential microtubule-based motor proteins travel along microtubules reaching into every corner of the cell. Mitotic kinesins play essential roles during all phases of mitosis. These proteins can be conceptualized as biological machines that transduce chemical energy into mechanical forces and motion. Kinesins use the energy derived from ATP hydrolysis to power their movement unidirectionally along microtubules and to transport molecular cargo to specific destinations. During mitosis, kinesins organize

microtubules into the bipolar structure that is the mitotic spindle. Kinesins mediate movement of chromosomes along spindle microtubules, as well as structural changes in the mitotic spindle associated with specific phases of mitosis. Experimental perturbation of mitotic kinesin function causes malformation or dysfunction of the mitotic spindle, frequently resulting in cell cycle arrest and cell death. It is rapidly becoming clear that mictrotubule motors play a crucial role in the functions of microtubules in mitosis.

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Among the mitotic kinesins which have been identified is Kinesin Spindle Protein (KSP). KSP belongs to the BimC family of 10 kinesins which are essentially a conserved kinesin subfamily of plus end-directed microtubule motors that assemble into bipolar homotetramers consisting of anti-parallel homodimers. Human KSP (also termed HsEg5) has been described [Blangy, et al., Cell, 83:1159-69 (1995); Whitehead, et al., Arthritis Rheum., 39:1635-42 (1996); Galgio et al., J. Cell Biol., 15 135:339-414 (1996); Blangy, et al., J Biol. Chem., 272:19418-24 (1997); Blangy, et al., Cell Motil Cytoskeleton, 40:174-82 (1998); Whitehead and Rattner, J. Cell Sci., 111:2551-61 (1998); Kaiser, et al., JBC 274:18925-31 (1999); GenBank accession numbers: X85137, NM004523 and U37426], and a fragment of the KSP gene (TRIP5) has been described [Lee, et al., Mol Endocrinol., 9:243-54 (1995); GenBank accession number L40372]. 20 Xenopus KSP homologs (Eg5), as well as Drosophila K-LP61 F/KRP 130 have been reported. KSP is a mitotic kinesin protein essential for proper DNA division in cells.

During mitosis KSP associates with microtubules of the mitotic spindle. Microinjection of antibodies directed against KSP into human cells prevents spindle pole separation during prometaphase, giving rise to monopolar spindles and causing mitotic arrest and induction of programmed cell death. The current model of KSP function in mitosis envisions that KSP and related kinesins in other, non-human organisms, bundle antiparallel microtubules and slide them relative to one another, thus forcing the two spindle poles apart. KSP may also mediate anaphase B spindle elongation and focussing of microtubules at the spindle pole. The mitotic spindle has been the subject of considerable research. The study of mitotic spindle proteins, such as microtubules, has yielded anti-mitotic compounds with important applications in cancer chemotherapy. The

demonstrated effectiveness of these anti-mitotic compounds in important medical and agricultural applications demonstrates the desirability of identifying and characterizing anti-mitotic compound development candidates.

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Because defects in the function of KSP have been implicated in cell cycle arrest, agents and/or compounds that modulate the activity of this kinesin will find use in the treatment of hyper-proliferative cell disorders such as cancer.

Medicaments generally exhibit their biological activities through strong interactions with their respective targets. Recently, advances in protein crystallography and computational chemistry have introduced a new method of structure-based drug design into the field of drug development. X-ray crystallography (crystallography) is an established, well-studied technique that provides what can be best described as a three-dimensional picture of what a molecule looks like in a crystal. Scientists have used crystallography to solve the crystal structures for many biologically important molecules. Many classes of biomolecules can be studied by crystallography, including, but not limited to, proteins, DNA, RNA and viruses.

Crystallography has been used extensively to view ligandprotein complexes for structure-based drug design. To view such complexes, known ligands are usually soaked into the target molecule crystal, followed by crystallography of the complex. Sometimes, it is necessary to cocrystallize the ligands with the target molecule to obtain a suitable crystal.

Given a "picture" of a target biomolecule or a ligand-protein complex, scientists can look for pockets or receptors where biological activity can take place. Thereafter, scientists can experimentally or computationally design high-affinity ligands (or drugs) for the protein/receptors. Computational methods have alternatively been used to screen for the binding of small molecules. This approach is also useful for developing new anti-mitotic agents.

Recently, independent efforts have confirmed the role of mitotic kinesins as critical mediators of microtubule organization during mitosis. It is postulated that blocking the biological function of motor proteins, e.g., human KSP, will lead to cell cycle arrest. While the binary

structure of KSP complexed with ADP has been published, (Turner et al., Journal of Biological Chemistry, 276; 25496-25502 (2001), no ternary structure of KSP complexed with a modulator, e.g., inhibitor, has heretofore been published. Consequently, until the present invention, which details the structural coordinates of human KSP with various ligands, albeit inhibitors, the identity and characterization of the novel binding site detailed herein was heretofore never available for rational drug design. As such, drug discovery efforts directed towards the KSP protein have been hampered by the lack of structural information about this protein and its complex with a ligand, e.g., monastrol. Such structural information would provide valuable information in discovery of anti-mitotic agents.

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The inventors provide herein crystals of KSP, complexed with a ligand, containing a novel, induced-fit binding site and have determined its three-dimensional structure. With this information, it is now possible, for the first time, to rationally design inhibitors of KSP, which can function as anti-mitotic agents, e.g. compounds which inhibit spindle pole separation during mitosis, thereby effectively inducing cell cycle arrest. It is believed that no one has heretofore reported determining the three-dimensional structure of the binding site identified herein.

Advantageous therapeutic embodiments would therefore comprise therapeutic and/or diagnostic agents based on or derived from the three-dimensional crystal structure of KSP including its novel binding site identified herein that have one or more than one of the functional activities of KSP. Additional therapeutic embodiments would comprise therapeutic and/or diagnostic agents based on or derived from molecular modeling of other members of the BimC protein family using the three-dimensional crystal structure of KSP and its binding site provided herein.

In accordance therewith, the novel-binding site disclosed herein is considered a potential target for anti-mitotic agents. In addition, the invention provides a process for creation of ligand candidate structures by means of a computer, using the structural coordinates of KSP's binding site provided herein. Furthermore, the information provided herein will enable one to search for ligand structures from a three-dimensional structure database containing known compounds.

SUMMARY OF THE INVENTION

The present invention is directed to the identification, characterization and three-dimensional structure of a novel ligand binding site of KSP. Binding of ligands to the novel binding site result in a conformational change in the three-dimensional structure of the protein and a modulation of the activity of KSP. This conformational change in turn results in the formation of a novel binding pocket in the KSP protein, which comprises the novel binding site of the instant invention. It has been further discovered that the formation of the novel binding pocket is facilitated by the concurrent binding of a nucleotide substrate or substrates to the protein. Moreover, the instant invention provides an attractive target for the rational design of potent and selective inhibitors of KSP identified by the methods of the invention, particularly new lead compounds useful in treating hyper-proliferative and KSP-dependent disorders.

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BRIEF DESCRIPTION OF THE DRAWINGS

FIGURE 1 An X-ray oscillation diffraction picture from a crystal of KSP in complex with (+)-monastrol and ADP (Compound 5-2b).

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FIGURE 2 The KSP-ADP-(+)-monastrol complex as shown in a ribbon presentation. The structure of the KSP-ADP-(+)-monastrol (Compound 5-2b) complex is shown in a ribbon representation. The bound conformations of ADP and Compound 5-2b are also given together with their respective electron density. The location of Compound 5-2b, the active isomer of monastrol, is seen at a novel induced-fit site, some 12Å distal from the nucleotide-binding site and catalytic center of the enzyme.

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FIGURE 3 (+)-Monastrol binding between helix-α2 and helix-α3. (+)-monastrol (Compound 5-2b) is seen to bind in between (the insertion loop of) helix-α2 and helix-α3 (which is immediately preceding the 'Switch 1' typically seen in all kinesins). Also shown are the side-chains of Arg119, Tyr211 and Trp127. The Arg119 and Tyr211 residues move upward and outward, yielding space to accommodate the binding of the

inhibitor. At the same time, the insertion loop of helix-α2 relocates its main-chain location with a downward shift of ~8Å; the side-chain of its Trp127 as a result swings inward by ~10Å, capping the entrance of the induced-fit cavity together with the side-chains of Arg119 and Tyr211. Lining the newly formed pocket and surrounding the inhibitor are residues 115-119, 127, 130, 132-134, 136, 137, 160, 211, 214, 215, 217, 218, 221 and 239.

FIGURE 4 Comparison between the binary and ternary

structure shown in ribbon presentation. The conformational alteration observed for the kinesin structure upon Compound 5-2b binding to the ADP-binary complex is not limited to the immediate vicinity of the inhibitor. Rearrangements of protein moieties are spread throughout the enzyme upon (+)-monastrol binding, including the switch I, switch II and neck linker region, with the exception that the nucleotide binding site of the protein as well as its β-sheet structure remaining basically unchanged.

FIGURE 5 Conformational alteration of KSP structure upon ligand binding shown in ribbon presentation. In the Switch I area of KSP, as circled, the main-chain re-orients its geometry significantly on both ends of Ala230. Although the helicity of the Switch I region is unchanged, the pitch at the C-terminal end of helix-α3 is increased in the ternary complex from that in the binary complex.

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25 FIGURE 6 Conformational alteration of KSP structure
upon ligand binding shown in ribbon presentation. In the Switch II region of
KSP, which is located on the opposite side of the binding site, as circled, the
C-terminal end of helix-α-4 is repositioned significantly. The tip of the
helix, in the Switch II region of KSP, near Arg305 is moved by ~6Å in the
ternary complex from its location in the binary complex.

FIGURE 7 <u>Conformational alteration of KSP structure</u> <u>upon ligand binding shown in ribbon presentation.</u> In the neck-linker region of KSP, which is the C-terminal portion of the protein construct, the residues

beginning from Lys357 to Phe362 swing by almost 180° in the ternary complex from its position in the ADP binary complex. Although residues 363–368 are present in the protein, they are disordered in the crystal and hence offer no electron density. The neck-linker region of KSP is circled. A close-up view is depicted, comparing the neck-linker region in the ternary complex to that in the binary complex.

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1-368.

FIGURE 8 Conformational alteration of KSP structure

upon ligand binding. A close-up view comparing the nucleotide-binding site
in the binary and ternary complexes of KSP is shown. Within experimental
errors, most of the backbone and side-chains for the two complexes in this
region of the protein can be super-positioned.

FIGURE 9 Motor Domain of Human KSP, Amino Acids

FIGURE 10 Binding Pocket of human KSP.

FIGURE 11 KSP/Compound 5-2b fluorescence data.

20 Compound 5-2b demonstrates a dose dependent decrease on the fluorescence of Trp127 in the presence of ADP or AMPPNP. These data indicate that the fluorescence assay is useful to measure potential KSP inhibitors. In the absence of the nucleotide, 5-2b does not cause a decrease on Trp127 fluorescence, suggesting the inability of 5-2b to bind to KSP in the absence of the nucleotide.

FIGURE 12 <u>KSP/Compound 8-1 fluorescence data.</u> Compound 8-1 demonstrates a dose dependent decrease on the fluorescence of Trp127 in the presence of ADP or AMPPNP. These data indicate that the fluorescence assay is useful to measure potential KSP inhibitors. In the absence of the nucleotide, 8-1 does not cause a decrease on Trp127 fluorescence, suggesting the inability of 8-1 to bind to KSP in the absence of the nucleotide.

FIGURE 13 KSP/Compound 1-7 fluorescence data.

Compound 1-7 demonstrates a dose dependent decrease on the fluorescence of Trp127 in the presence of ADP or AMPPNP. These data indicate that the fluorescence assay is useful to measure potential KSP inhibitors. In the absence of the nucleotide, 1-7 does not cause a decrease on Trp127 fluorescence, suggesting the inability of 1-7 to bind to KSP in the absence of the nucleotide.

FIGURES 14A and 14B KSP Inhibitor Pharmacophore Models.

10 The two pharmacophore models derived from analysis and further computational processing of the crystallized complex are illustrated. Spheres represent a center of a hydrophobic group and boxes represent either a hydrogen bond acceptor (HA) or hydrogen bond donor (HD). All distances are in Å.

FIGURE 15 KSP Inhibitor Pharmacophore Models in KSP Binding

Site. A schematic view of the two pharmacophore models superimposed and mapped onto the ligand binding site of KSP defined, in part, by the amino acids of Figure 10.

Only relevant KSP protein residues are shown.

20 FIGURE 16 KSP Inhibitor Pharmacophore Model.

A pharmacophore model derived from analysis and further computational processing of a crystallized complex is illustrated. Spheres represent a center of a hydrophobic group and boxes represent either a hydrogen bond acceptor (HA).

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TABLE 1 KSP motor domain/Compound 5-2b X-ray coordinates.

TABLE 2 KSP motor domain/Compound 1-7 X-ray

30 coordinates.

TABLE 3 KSP motor domain/Compound 2-7 X-ray coordinates.

TABLE 4 KSP motor domain/Compound 4-2a X-ray

TABLE 5 Novel KSP ligand binding site/Compound 5-

5 2b X-ray coordinates.

coordinates.

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DETAILED DESCRIPTION OF THE INVENTION

"Conservative substitutions" are those amino acid substitutions which are functionally equivalent to the substituted amino acid residue, either by way of having similar polarity, steric arrangement, or by belonging to the same class as the substituted residue (e.g., hydrophobic, acidic or basic), and includes substitutions having an inconsequential effect on the three-dimensional structure of KSP with respect to the use of said structure for the identification and design of KSP or KSP complex inhibitors, for molecular replacement analyses and/or for homology modeling.

Amino acid sequence "similarity" is a measure of the degree to which aligned amino acid sequences possess identical amino acids or conservative amino acid substitutions at corresponding positions.

A "fragment" of KSP is meant to refer to a protein molecule which contains a portion of the complete amino acid sequence of the wild type or reference protein.

As used herein, a "variant" of a KSP protein refers to a polypeptide having an amino acid sequence with one or more amino acid substitutions, insertions, and/or deletions compared to the sequence of the invention receptor protein.

Generally, differences are limited so that the sequences of the reference (native or wild type KSP) and the variant are closely similar overall, and in many regions, identical. Such variants are generally biologically active and necessarily have less than 100% sequence identity with the polypeptide of interest.

Preferably, the biologically active variant KSP has an amino acid sequence sharing at least about 80% amino acid sequence identity with the reference KSP, preferably at least about 85%, more preferably at least about 90%, and most preferably at least about 95%. Amino-acid substitutions are preferably substitutions of single amino-acid residues. Preferably, such polypeptides also possess characteristic structural features and biological activity of a native KSP polypeptide.

For example, variants of KSP are characterized as containing key functional residues that participate in ligand binding. These polypeptide fragments, in turn, have been derivatized by methods akin to traditional drug development. Preferred polypeptides and polynucleotides of the present invention are expected to have, *inter alia*, similar biological functions/properties to their homologous polypeptides and polynucleotides. Furthermore, preferred polypeptides and polynucleotides of the present invention have at least one GPR25 activity.

Sequence similarity or percent similarity can be determined, for example, by comparing sequence information using sequence analysis software such as the GAP computer program, version 6.0, available from the University of Wisconsin Genetics Computer Group (UWGCG). The GAP program utilizes the alignment method of Needleman and Wunsch (J. Mol. Biol. 48:443, 1970), as revised by Smith and Waterman (Adv. Appl. Math. 2:482, 1981).

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As used herein, a "binding site" refers to a region of a molecule or molecular complex that, as a result of its shape and charge potential, favorably interacts or associates with another agent (including, without limitation, a protein, polypeptide, peptide, nucleic acid, including DNA or RNA, molecule, compound, antibody or drug) via various covalent and/or non-covalent binding forces.

The terms "ligand binding site" and "binding site" are used interchangeably and refer to a region of a human KSP resulting from the complex of a ligand with KSP. It is believed that this ligand binding site, as a result of its shape and charge potential, favorably interacts or associates with a ligand or binding partner, which is preferably an inhibitor of KSP function. The binding of the ligand to this binding site induces global conformational changes to the KSP protein, thereby potentially modulating the mitotic activity of the protein and thereby inhibiting cell division and facilitating cell cycle arrest. A ligand binding site according to the present invention may include, for example, the actual site of any one of the herein disclosed compounds binding with KSP, as well as any other moiety - chemical or biological - which preferably inhibits the activities of KSP by binding to the ligand binding site disclosed herein.

As used herein, the terms "bind" and "binding" when used to describe the interaction of a ligand with a binding site or a group of amino acids means that the binding site or group of amino acids are capable of forming a covalent or non-covalent bond or bonds with the ligand.

Preferably, the binding between the ligand and the binding site or amino acid(s) is non-covalent. Such a non-covalent bond includes a hydrogen bond, an electrostatic bond, a van der Waals bond or the like. The binding of the ligand to the binding site may also be characterized by the ability of the ligand to co-crystallize with KSP within the novel binding pocket of the instant invention. It is further understood that the use of the terms "bind" and "binding" when referring to the interaction of a ligand with the novel binding site of the instant invention includes the covalent or non-covalent interactions of the ligand with all or some of the amino acid residues comprising the binding site.

A "KSP complex" refers to a co-complex of a molecule/complex comprising the KSP in bound association with a ligand either by covalent or non-covalent binding forces at the binding site disclosed herein. A non-limiting example of a KSP complex includes KSP-(+)-monastrol, or KSP bound to any one of the compounds listed herein.

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The present invention relates to the three-dimensional structure of ligand bound-KSP or of a KSP analogue, and more specifically, to the structure of KSP's binding site as determined using X-ray crystallography and various computer modeling techniques. The coordinates of KSP bound to ADP and one of the ligand compounds described herein as shown in Tables 1-4 (relating to the entire motor domain), are useful for a number of applications, including, but not limited to, the characterization of a three-dimensional structure of KSP including its novel binding site, as well as the visualization, identification and characterization of a KSP ligand binding site. The ligand binding site structure(s) may then be used to predict the orientation and binding affinity of a designed or selected inhibitor of KSP, a KSP analogue or of a KSP complex. In general, KSP structures referred to herein are the KSP-ligand bound conformation of KSP. As an example, when referring to an antibody specific for the KSP of the invention, it means an antibody having an affinity for the KSP-ligand bound conformation disclosed herein.

In particular, the invention is drawn to the three-dimensional structure of a ligand bound KSP e.g., when bound to a ligand, preferably an inhibitor.

The amino acid sequence of the motor domain of human KSP is depicted in SEQ ID NO:1. These amino acids correspond to residues 1-368 of the native protein. Another aspect of the invention is a substantially pure isolated amino acid of the amino acid sequence set forth in SEQ ID NO:1. Another aspect of the invention is a variant of that isolated amino acid. Preferably the variant of the amino acid of SEQ ID NO:1 comprises one or more amino acid substitution(s) or deletion(s) of one or more of the amino acids that form the novel binding pocket of the instant invention. More preferably the variant of the amino acid of SEQ ID NO:1 comprises an amino acid substitution of one of the amino acids which form the novel binding pocket of the instant invention.

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Another aspect of the invention is an isolated variant of KSP wherein the variant comprises one or more amino acid substitution(s) or deletion(s) of one or more of the amino acids that form the novel binding pocket of the instant invention. More preferably the variant of KSP comprises an amino acid substitution of one of the amino acids which form the novel binding pocket of the instant invention.

The KSP of the invention preferably comprises a ligand binding site characterized by the amino acid residues as set forth in Figure 10 or the relative structural coordinates of those amino acid residues according to Tables 1-4 ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 2.0 Å (or more preferably, not more than about 1.0 Å, and most preferably, not more than about 0.5 Å). It is understood that the amino acids listed above represent the residues defining the novel binding pocket formed upon the complexation of a ligand of the invention with KSP. It is further understood that specific binding interactions between the listed residues may or may not occur based on the size of the ligand and structure of the ligand. It is also understood that the computational length of the allowable van der Waals interactions is also a factor when determining whether an amino acid residue binds to a ligand. It is therefore understood that the binding of a ligand of the instant invention may take place between those residues listed in Figure 10 or a subset thereof.

It has been surprisingly discovered that compounds previously disclosed as kinesin inhibitors, and other recently identified

inhibitors of KSP, bind to the KSP protein at the novel binding site described herein. In particular, (+)-monastrol (Compound 5-2b), a compound previously described as inhibiting KSP kinesin activity (see Mayer, T. U. et al. Science 286:971 (1999)) has been found to be a ligand of the novel binding site of the invention. Inhibitors of KSP have also been disclosed in pending U.S. provisional applications Ser. Nos. 60/344,453 (Case 20990PV), 60/338,383 (Case 20995PV), 60/338,380 (Case 20996PV), 60/338,779 (Case 20997PV), 60/338,344 (Case 20998PV), 60/338,379 (Case 20999PV), 60/362,922 (Case 21047PV), 60/383,449 (Case 21018PV), 60/383,478 (Case 21060PV), 60/388,621 (Case 21114PV, filed June 14, 2002) and 60/388,828 (Case 21119PV, filed June 14, 2002). Additionally, inhibitors of KSP kinesin activity are described in PCT Publications WO 01/30768 and WO 01/98278.

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The 3-dimensional structure of KSP, bound with Mg⁺⁺-ADP and Compound 5-2b, was determined at 2.5Å resolution. Compound 5-2b was found to bind to KSP via an induced-fit some 12Å away from the catalytic center of the enzyme, resulting in the creation of a previously unknown binding pocket that is non-existent in the absence of Compound 5-2b (or the other ligands described herein). The binding of Compound 5-2b also introduced significant alteration to the structural conformation in other regions of the KSP motor protein, with the interesting exception that the nucleotide-binding pocket was virtually unaltered from that seen in the ADP binary complex. An analysis of the temperature-factor distribution in the ADP binary and ADP/5-2b ternary complexes of KSP revealed that the protein region surrounding the induced-fit binding pocket of 5-2b became highly rigid upon 5-2b binding.

Using the seeding method, high quality single crystals were obtained for KSP prepared in the presence of ADP and 5-2b. A diffraction data set to 2.5Å resolution was collected and processed in the orthorhombic P2₁2₁2₁ space group. The R_{sym} was 0.084 and the data completeness was 99%. The cell dimensions were 69.5Å, 79.5Å and 159.0Å. An oscillation X-ray diffraction picture of a KSP crystal is given in Figure 1.

The 3-dimensional, tertiary structure of KSP, bound with Mg⁺⁺-ADP and 5-2b, was determined at 2.5Å resolution with use of phases derived from a combination of molecular replacement, extensive manual

rebuilding, and dynamic refinement. Two identical protein complexes were found in the asymmetric unit of the crystal and were related by a local, non-crystallographic 2-fold axis. For each, the electron density of the protein as well as those of the ligands (ADP, Mg⁺⁺, and 5-2b) was all well defined. 5-2b was seen to be of the S handedness. Residues 2-17, 272-286, and 363-368 were disordered and showed no electron densities (The N-terminal Met1 residue was processed upon expression).

The structure of the KSP/ADP/Compound 5-2b complex is shown (Figure 2) in a ribbon representation. The bound conformations of ADP and 5-2b are also given together with their respective electron density. The location of 5-2b is seen at a novel induced-fit site, some 12Å distal from the nucleotide-binding site and catalytic center of the enzyme. An enlarged section of this region is shown in Figure 3, together with 5-2b.

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In Figure 3 the Compound 5-2b is seen to bind in between (the insertion loop of) helix-α2 and helix-α3 (which is immediately preceding the 'Switch 1' typically seen in all kinesins). Also shown are the side-chains of Arg119, Tyr211 and Trp127. The Arg119 and Tyr211 residues move upward and outward, yielding space to accommodate the binding of the inhibitor. At the same time, the insertion loop of helix-α2 relocates its main-chain location with a downward shift of ~8Å; the side-chain of its Trp127 as a result swings inward by ~10Å, capping the entrance of the induced-fit cavity together with the side-chains of Arg119 and Tyr211. Lining the newly formed pocket and surrounding the inhibitor are the amino acid residues listed in Figure 10. A comparison of this region in the binary and ternary complex is given in Figure 4.

The binding pocket of Compound 5-2b is novel and not previously known, insofar that this binding site does not exist until an inhibitor binds. Hence, this pocket is "induced-fit" by a ligand such as Compound 5-2b. This allosteric binding pocket, located away from the nucleotide-binding site of the motor protein, is not restricted to Compound 5-2b, but is also observed upon the crystal structure determination of complexes of KSP with other compounds of diverse chemical structure that are inhibitors of KSP activity. These results have a profound impact on the design of non-active-site directing inhibitors of KSP.

In a further embodiment of the invention is a method of causing a conformational alteration in the structure of KSP by exposing the KSP to a ligand of the novel ligand binding site of the instant invention.

The conformational alteration observed for the kinesin structure upon

Compound 5-2b binding (and the binding of other compounds) to the ADP-KSP binary complex is not limited to the immediate vicinity of the inhibitor. Rearrangements of protein moieties are spread throughout the enzyme upon 5-2b binding, with the exception that the nucleotide binding site of the protein as well as its β-sheet structure remain basically unchanged. Among the changes away from the induced-fit pocket, three are noteworthy:

1. In the Switch I area of KSP, as circled in Figure 5 and in a close-up view, the main-chain re-orients its geometry significantly on both ends of Ala230. It can be seen that although the helicity of the Switch I region is unchanged, the pitch at the C-terminal end of helix-α3 is increased in the ternary complex from that in the binary complex.

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- 2. In the Switch II region of KSP, which is located on the opposite side of the 5-2b binding site as circled in Figure 6 and in a close-up view, the C-terminal end of helix- α 4 is repositioned significantly. The tip of this helix near Arg305 is moved by ~6Å in the ternary complex from its location in the binary complex.
- 3. In the neck-linker region of KSP, which is the C-terminal portion of our protein construct, the residues beginning from Lys357 to Phe362 swing by almost 180° in the ternary complex from its position in the ADP binary complex. Although residues 363–368 are present in our protein, they are disordered in the crystal and hence offer no electron density. The neck-linker region of KSP is circled in Figure 7. A close-up view is depicted comparing this region in the ternary complex to that in the binary complex.

In addition to these changes, there are other smaller regional repositionings of main-chains and side-chains of the protein. Most interestingly, the nucleotide-binding site of the motor protein, where ATP hydrolysis occurs, is basically unaltered upon 5-2b binding. A close-up view comparing this site in the binary and ternary complexes of KSP is shown in Figure 8. Within experimental errors, most of the backbone and

side-chains for the two complexes in this region of the protein can be superimposed.

The effect of overall conformational changes induced by Compound 5-2b could also be examined by comparing the distribution of temperature factors.

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High quality single crystals were also obtained for other compounds that are inhibitors of KSP. 3-Dimensional structure determined at 2.5 Å with those crystals demonstrated that the other inhibitor compounds also induce-fit into the protein in the same manner as compound 5-2b.

Consequently, an embodiment of the invention provides protein crystals of KSP complexed with a ligand bound to the ligand binding site disclosed herein and methods for making KSP or a KSP homolog. The crystals provide means to obtain atomic modeling information of the specific amino acids and their atoms forming the binding site and that interact with molecules e.g., ligands or binding partners that bind to the KSP, via the binding site.

The crystals also provide modeling information regarding the protein-ligand interaction, as well as the structure of ligands bound thereto. The KSP crystal or a KSP homolog according to the present invention can be obtained by crystallizing it with a material or compound or molecule which binds to the herein disclosed binding site of the KSP. The KSP crystal according to the present invention includes KSP (human Eg5) and the material which binds to the specific binding site of KSP.

Preferred crystalline compositions of this invention are capable of diffracting X-rays to a resolution of better than about 3.5 Å, and more preferably to a resolution of about 2.6 Å or better, and even more preferably to a resolution of about 2.0 Å or better, and are useful for determining the three-dimensional structure of the material. (The smaller the number of angstroms, the better the resolution.)

The relative structural coordinates of the amino acid residues of the KSP motor domain, when the X-ray diffraction is obtained for the crystalline complex of KSP and a ligand compound described herein, are shown in Tables 1-4.

In another aspect, the present invention provides the threedimensional structure of human KSP as well as the identification and

characterization of a binding site there within. The identification of this site permits design and identification of compounds that bind to the ligand binding site and modulate KSP related activities. The compounds include inhibitors which specifically inhibit cell proliferation.

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Of equal import is the fact that knowledge of the threedimensional structure of the binding site of KSP provides a means for investigating the mechanism of action of the protein and tools for identifying inhibitors of its function.

As used herein, a ligand binding site also includes KSP or KSP analog residues which exhibit observable NMR perturbations in the presence of a binding ligand, such as any one of the herein disclosed inhibitors or any other ligand. While such residues exhibiting observable NMR perturbations may not necessarily be in direct contact with or immediately proximate to ligand binding residues, they may be critical to KSP residues for rational drug design protocols.

For example, knowledge of the three-dimensional structure of the ligand binding site allows one to design molecules, preferably pharmaceutical agents, capable of binding thereto, including molecules which are thereby capable of inhibiting the interaction of KSP with its native ligands, thereby inducing cell arrest.

Assays may be performed and the results analyzed to determine whether the agent is an inhibitor (i.e., the agent may reduce or prevent binding affinity between KSP and its native ligand/binding partner), or has no effect on the interaction between KSP and its native ligand. Agents identified using the foregoing methods, and preferably inhibitors of KSP, may then be tested as therapeutics in the treatment and/or prevention of hyper-proliferative cell disorders and other diseases that are also characterized by the presence of the hyper-proliferative cells such as cancer.

Once a KSP binding agent/inhibitor has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or side groups in order to improve or modify its selectivity and binding properties – that is its affinity for the ligand binding site disclosed herein. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. Such substituted chemical compounds may then be analyzed for efficiency of fit the ligand binding site of KSP by the same computer methods described in detail above.

Various molecular analysis and rational drug design techniques are further disclosed in U.S. Pat. Nos. 5,834,228, 5,939,528 and 5,865,116, as well as in PCT Application No. PCT/US98/16879, published as WO 99/09148, the contents of which are hereby incorporated by reference.

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In another aspect of the instant invention, the high quality single crystals of the KSP complexes comprising the KSP, ADP and the compounds described herein could be used to obtain single crystals of a KSP complex which comprises a compound that weakly binds to KSP or one or more weakly binding fragments of a compound that binds to KSP. This method may be termed intra-crystal ligand exchange. Thus, for example and not limiting in the scope of this embodiment, high quality single crystals of KSP-ADP-Compound 5-2b complex are exposed to the crystallization buffer described in the Materials and Methods which further contains 1mM of a test compound that weakly binds to KSP. It is expected that the test compound will intercalate into the crystal and replace the compound 5-2b in the binding site. One or more molecular fragments of compounds that strongly bind to KSP may also be utilized in this technique.

X-ray diffraction data may be collected (as described in the Materials and Methods) from the high quality single crystals obtained by the intra-crystal ligand exchange technique. The 3-dimensional, tertiary structure of KSP bound to such a weakly binding compound could be utilized to guide the structural modification of the compound and, as a result, optimize the binding of the modified compound to KSP. The 3-dimensional tertiary structure of KSP bound to molecular fragment(s) could be utilized to guide in the identification of a new template for a compound having optimal binding to KSP.

Once the material is designed or selected, the affinity of the material to

KSP may be calculated. For the inhibitor to be effective, it should have a high affinity for the ligand binding site, low energy difference between that energy calculated before and after binding. The affinity of the inhibitor may be measured by calculating the dissociation constant of the complex of KSP and the inhibitor. The dissociation constant is preferably 100 micromoles or less. The inhibitor preferably also maintains the bonding with KSP stably after binding. In order to do this, electrostatic repulsion such as charge-charge interactions, dipole-dipole and charge-dipole interactions between the inhibitor and KSP should not occur or be minimized. The sum of

electrostatic interaction should be neutral or give a positive effect to the enthalpy of the bonding. Examples of programs designed for calculating such affinity include, but

are not limited to as follows: Gaussian 92, revision C [M. J. Frisch, Gaussian, Inc., Pittsburgh, Pa. © 1992]; AMBER, version 4.0 [P. A. Kollman, University of California at San Fransisco, © 1994]; QUANTA/CHARMM [Molecular Simulations, Inc., Burlington, Mass. © 1994]; and Insight II/Discover (Biosysm Technologies Inc., San Diego, Calif., © 1994). Using the lead compound selected by the method, a stronger inhibitor can be made or designed. This process will be described below.

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As well, any compound or anti-mitotic agent (lead compound) selected or designed in accordance with the methods disclosed herein can be changed or modified. Atoms, substituents or a part of the structure may be altered to increase the binding affinity to KSP. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. It is noted that components known in the art to alter conformation should be avoided. The substituted chemical compounds may then be analyzed for fit with KSP by the same computer methods described herein.

After the material designed by the computer method described above is prepared and bound to KSP to produce a crystal, the 3-dimensional structure of the complex may be determined at high enough resolution (over 0.28 nm) using X-ray crystallographic methods. The information gained therefrom e.g., about the interaction between KSP and the inhibitor obtained from this can then be used to modify the inhibitor and to increase the affinity of the inhibitor for the ligand binding site of KSP.

Thus, for example, those atoms considered to be involved in binding to the ligand binding site of KSP disclosed herein can be mutated by exchanging one or more of the amino acid residues in the ligand binding site or in the motor domain of KSP that eventually effects the function of KSP on the underlying cell. As an example, if a cell's hyper-proliferative state is not effected by the mutated KSP, it may be surmised that the mutation very likely has not affected the function of KSP. In the alternative scenario, where the mutation decreases the hyper-proliferative state of the diseased cell, then one may surmise that the mutation has affected the ability of KSP to function in its intended purpose, e.g. hydrolyze ATP to ADP or bind microtubule etc. due to the substitution of the amino acid residue. This method can be used to identify amino acid residues in the original KSP which are important in the binding of the ligand to the binding site of KSP disclosed herein.

Once the amino acid residues in the ligand binding site of KSP have been identified as involved in the overall function attending KSP, the structure of the binding site can be identified based on the three-dimensional structure of KSP. Based on the structure of the binding site, a compound such as a peptide or other compound can be screened and designed which will fit into the three-dimensional model of the binding site.

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Likewise, just as the three-dimensional modeling of KSP is provided by the present invention using the coordinates from the X-ray defraction patterns, these can be either analyzed directly to provide the three-dimensional structure (if of sufficiently high resolution). Alternatively, the atomic coordinates for the crystallized KSP, as provided herein, can be used for structure determination. The X-ray diffraction patterns obtained by methods of the present invention, can be provided on computer readable media, and used to provide electron density maps.

The electron density maps, provided by analysis of the X-ray coordinates of KSP complexed with Compound 5-2b, provided herein, may then be fitted using suitable computer algorithms to generate secondary, tertiary and/or quaternary structures and/or domains of KSP, which structures and/or domains are then used to provide an overall three-dimensional structure, as well as binding and/or active sites of KSP.

Knowledge obtained concerning KSP including the binding site defined herein can also be used to model the tertiary structure of related kinesin proteins, in particular members of the BimC protein family.

As an example, the structure of renin has been modeled using the tertiary structure of endothiapepsin as a starting point for the derivation. Model building of cercarial elastase and tophozoite cysteine protease were each built from known serine and cysteine proteases that have less than 35% sequence identity. The resultant models were used to design inhibitors in the low micromolar range. (Proc. Natl. Acad. Sci. 1993, 90, 3583).

Furthermore, alternative methods of tertiary structure determination that do not rely on X-ray diffraction techniques and thus do not require crystallization of the protein, such as NMR techniques, are simplified if a model of the structure is available for refinement using the additional data gathered by the alternative technique. Thus, knowledge of the tertiary structure of the KSP binding site provides a significant window to the

structure of the other kinesin family members. Thus, an embodiment of this invention envisions use of atomic coordinates of KSP protein, or fragment, analog or variant thereof, to model a KSP protein.

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One skilled in the relevant art may use conventional molecular modeling methods to identify a ligand binding site of a KSP of another species. Specifically, coordinates provided by the present invention may be used to characterize a three-dimensional structure of the target KSP molecule, liganded or unliganded. Importantly, such a skilled artisan may, from such a structure, computationally visualize a putative binding site and identify and characterize other features based upon the coordinates provided herein. Such putative ligand binding sites may be further refined using chemical shift perturbations of spectra generated from various and distinct KSP complexes, e.g. from other species, competitive and non-competitive inhibition experiments, and/or by the generation and characterization of KSP or ligand mutants to identify critical residues or characteristics of the ligand binding site.

Such identification of a putative ligand binding site is of great import in rational drug design.

It is noted that in order to use the structural coordinates generated from the complex KSP described herein in Tables 1-4, it may be necessary to display the relevant coordinates as, or convert them to, a three-dimensional shape or graphical representation, or to otherwise manipulate them. In general, such a three-dimensional representation of the structural coordinates will find use in rational drug design, molecular replacement analysis, homology modeling, and mutation analysis. This is typically accomplished using any of a wide variety of commercially available software programs capable of generating three-dimensional graphical representations of molecules or portions thereof from a set of structural coordinates. The scientific art is replete with conventional software programs, which are incorporated by reference herein in their entirety. Refer to, for example, GRID (Oxford University, Oxford, UK); AUTODOCK (Scripps Research Institute, La Jolla, Calif.); Flo99 (Thistlesoft, Morris Township, N.J.) etc.

For storing, transferring and using such programs, a machine, such as a computer, is also contemplated, which produces a three-

dimensional representation of the KSP binding site. The machine would comprise a machine-readable data storage medium comprising a data storage material encoded with machine-readable data. Machine-readable storage media comprising data storage material include conventional computer hard drives, floppy disks, DAT tape, CD-ROM, and other magnetic, magnetooptical, optical, floptical and other media which may be adapted for use with a computer. The machine further comprises a working memory for storing instructions for processing the machine-readable data, as well as a central processing unit (CPU) coupled to the working memory and to the machinereadable data storage medium for the purpose of processing the machinereadable data into the desired three-dimensional representation. As well, the machine of the present invention further comprises a display connected to the CPU so that the three-dimensional representation may be visualized by the user. Accordingly, when used with a machine programmed with instructions for using said data, e.g., a computer loaded with one or more programs of the sort identified above, the machine provided for herein is capable of displaying a graphical three-dimensional representation of the KSP complex described herein and set forth in Tables 1-4.

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The structural coordinates of the present invention enable one to use various molecular design and analysis techniques in order to (i) solve the three-dimensional structures of related molecules, preferably molecular complexes such as those of other species or members of BimC family of proteins; as well as (ii) design, select, and synthesize chemical agents capable of favorably associating or interacting with a ligand binding site of a KSP molecule, wherein the molecular chemical entity would preferably inhibit KSP function including inducing mitotic arrest in cells contacted therewith.

Thus, the present invention provides a method for determining the molecular structure of a molecular complex whose structure is unknown, comprising the steps of obtaining the molecular complex whose structure is unknown, e.g., from a related species, and then generating NMR data there from. The NMR data from the molecular complex whose structure is unknown can then be compared to the structure data obtained from the KSP complex of the present invention. Then, 2D, 3D and 4D isotope filtering, editing and triple resonance NMR techniques can be used to conform the 3D structure described

herein for the KSP complexes disclosed in Tables 1-4 to the NMR data from unknown target molecular complex. Alternatively, molecular replacement may be used to conform the 3D structure of the present invention to X-ray diffraction data from crystals of the unknown target molecular complex.

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Molecular replacement involves correctly orienting and positioning the known structure into the crystal unit cell of the unknown structure. This is accomplished by a six dimensional (three positional and three rotational) search process that involves computation of a set of theoretical diffraction data using the known structure for every orientation and position searched and comparing it with the observed diffraction data of the unknown structure. The best match defines the correct position and orientation of the known structure in the unknown unit cell. This match offers phase information for use in conjunction with X-ray diffraction data of the unknown structure for the determination of its 3-dimensional structure.

In another aspect, this invention envisions use of atomic coordinates of the KSP protein disclosed herein, to design a chemical compound capable of associating with KSP or a fragment, analog or variant thereof.

For example, one method of this invention for evaluating the ability of a chemical entity to associate with any of the proteins or protein-ligand complexes set forth herein comprises the steps of: a) employing computational means to perform a fitting operation (docking) between the chemical entity and a binding pocket or other surface feature of the molecule or molecular complex; and b) analyzing the results of said fitting operation to quantify the association between the chemical entity and the binding pocket.

In another aspect, the invention envisions use of atomic coordinates of the KSP protein to design a model of ligands in the binding site defined herein.

Preferred embodiments of the aforementioned uses are those wherein the KSP protein comprises a binding site characterized by amino acid residues as set forth in Figure 10.

As a general rule, one may use knowledge of the geography of the various regions of the ligand binding site disclosed herein, e.g. hydrophobic and/or hydrophilic to design KSP analogs (mutant) in which

the overall KSP structure is not changed, but change does affect biological activity ("biological activity" being used here in its broadest sense to denote function). Thus, one may make changes to the amino acid sequences to effectively obtain a KSP analog/mutant that exhibits a greater affinity for its binding ligand. As well, one may correlate biological activity to structure. If the structure is not changed, and the mutation has no effect on biological activity, then the mutation has no biological function. If, however, the structure is not changed and the mutation does affect biological activity, then the residue (or atom) is essential to at least one biological function.

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Similar molecular modeling is also provided by the present invention for rational drug design (RDD) of mimetics and ligands of KSP, "ligand" being used in the broadest sense, referring to any substance capable of observable binding to the KSP protein at the herein disclosed binding site. The drug design paradigm uses computer modeling programs to determine potential mimetics and ligands which are expected to interact with sites on the protein. The potential mimetics or ligands are then screened for activity and/or binding. For KSP-related mimetics or ligands, screening methods can be selected from assays for at least one biological activity of KSP, e.g., antimitotic activity. Thus, an embodiment of the invention envisions use of the structural information from the ligand/protein complexes found herein including the information derived therefrom in designing new chemical or biological moieties that bind tighter, bind more specifically, have better biological activity or have better safety profile than known ligands that bind KSP.

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The computer modeling method disclosed herein can also be used to remodel the mimetics or ligands to improve the affinity or solubility, and produce an optimized pharmaceutical agent.

The resulting optimized mimetics or ligands can thereafter be prepared and the inhibitory activity for KSP can be tested *in vitro* and *in vivo*. If the test confirms that the material does indeed inhibit KSP, then the material or a derivative can be used as an anti-mitotic agent. Using the method as described above, the compound identified to have inhibitory activity may thereafter be used as a lead compound to obtain an improved inhibitor.

In order to confirm the affinity predicted by the computer modeling method, the dissociation constant of the complex may be experimentally measured.

The resulting mimetics or ligands are then provided by methods of the present invention and are useful for treating, inhibiting or preventing KSP-modulated diseases in animals, including humans.

Preferably the ligands of the novel binding site provided herein are useful in the treatment or prevention of a hyper-proliferative disease, preferably cancer. Preferably, the ligand(s) identified by the methods described herein are useful in the treatment of cancer.

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The ligands identified by the methods of this invention may be administered to mammals, preferably humans, either alone or, preferably, in combination with pharmaceutically acceptable carriers, excipients or diluents, in a pharmaceutical composition, according to standard pharmaceutical practice. The ligands can be administered orally or parenterally, including the intravenous, intramuscular, intraperitoneal, subcutaneous, rectal and topical routes of administration.

As used herein, the term "composition" is intended to encompass a product comprising the specified ingredients in the specific amounts, as well as any product which results, directly or indirectly, from combination of the specific ingredients in the specified amounts.

The pharmaceutical compositions containing the active ingredient may be in a form suitable for oral use, for example, as tablets, troches, lozenges, aqueous or oily suspensions, dispersible powders or granules, emulsions, hard or soft capsules, or syrups or elixirs. When a ligand according to this invention is administered into a human subject, the daily dosage will normally be determined by the prescribing physician with the dosage generally varying according to the age, weight, sex and response of the individual patient, as well as the severity of the patient's symptoms.

In one exemplary application, a suitable amount of a ligand of the novel KSP ligand binding site is administered to a mammal undergoing treatment for cancer. Administration occurs in an amount between about 0.1 mg/kg of body weight to about 60 mg/kg of body weight per day, preferably of between 0.5 mg/kg of body weight to about 40 mg/kg of body weight per day.

Consequently, an object of the invention is to provide a method for determining the three-dimensional structure of a protein containing the ligand binding site as disclosed herein, or a complex of the protein with a ligand thereof, using homology modeling techniques and structural coordinates for a composition of this invention. Homology modeling involves constructing a model of an unknown structure using structural coordinates of one or more related proteins, protein domains and/or subdomains. Homology modeling may be conducted by fitting common or homologous portions of the protein or peptide whose three-dimensional structure is to be solved to the three-dimensional structure of homologous structural elements. Homology modeling can include rebuilding part or all of a three-dimensional structure with replacement of amino acids (or other components) by those of the related structure to be solved.

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One of the objects of this invention is to provide threedimensional structural information on new complexes of BimC family 15 members of which KSP is a member with various ligands, as well as muteins or other variants of any of the foregoing. To that end, the invention provides for the use of the structural coordinates of a crystalline composition of this invention, or portions thereof, to solve, e.g., by molecular replacement, the three-dimensional structure of a crystalline form 20 of such a ligand-protein complex, typically involving a protein containing at least one ligand binding site as disclosed herein. Doing so involves obtaining X-ray diffraction data for crystals of the protein-ligand complex for which one wishes to determine the three-dimensional structure. Then, one determines the three-dimensional structure of that protein or complex by 25 analyzing the X-ray diffraction data using molecular replacement techniques with reference to the previous structural coordinates. As described in U.S. Pat. No. 5,353,236, for instance, molecular replacement uses a molecule having a known structure as a starting point to model the structure of an unknown crystalline sample. 30

Still further, the invention also includes compositions and methods for identifying binding sites of other members of the BimC protein family. The methods involve examining the surface of a protein of interest, preferably a kinesin, to identify residues that facilitate binding to the binding site. The residues can be identified by homology to the ligand binding site of

human KSP described herein. Overlays and super-positioning with a threedimensional model of a KSP binding site, or a portion thereof that contains a ligand binding site, also can be used for this purpose.

An alternative method of this invention provides for selecting from a database of chemical structures a compound capable of binding to a BimC family protein. The method starts with structural coordinates of a crystalline composition of the invention, e.g., coordinates defining the three-dimensional structure of a BimC family protein or a portion thereof e.g., the herein provided coordinates relative to human KSP.

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Points associated with that three-dimensional structure are characterized with respect to the extent of favorable interactions with one or more functional groups. A database of chemical structures is then searched for candidate compounds containing one or more functional groups disposed for favorable interaction with the protein based on the prior characterization.

15 Compounds having structures which best fit the points of favorable interaction with the three-dimensional structure are thus identified.

An exemplary embodiment of the invention provides methods for identifying and designing small molecules that bind to the binding site using atomic models of KSP provided herein. The method involves modeling test compounds that fit spacially into the binding site of interest using an atomic structural model comprising a KSP binding site or portion thereof, screening the test compounds in a biological assay characterized by binding of a test compound to KSP, and identifying a test compound that binds to KSP.

Also provided is a method for identifying a potential inhibitor of KSP, comprising the steps of using a three-dimensional structure of a KSP binding site as defined by the relative structural coordinates set forth in Table 5 or the relative structural coordinates of the amino acids of Figure 10 as set forth in Tables 1-4 to design or select a potential inhibitor, and obtaining or synthesizing said potential inhibitor. The inhibitor may be selected by screening an appropriate database, may be designed de novo by analyzing the steric configurations and charge potentials of an empty KSP binding site in conjunction with the appropriate software programs, or may be designed using characteristics of known inhibitors to create "hybrid" inhibitors. The inhibitor may then be contacted with KSP, and the effect of

the inhibitor on KSP related function may be assessed. For instance, a potential inhibitor identified by this method may be contacted with KSP in the presence of one or two KSP substrates selected from ATP and microtubules, and determining the effect the potential inhibitor has on KSP ATPase activity. It is also within the confines of the present invention that a potential inhibitor may be designed or selected by identifying chemical entities or fragments capable of associating with KSP; and assembling the identified chemical entities or fragments into a single molecule to provide the structure of the potential inhibitor.

In furtherance of the above, there is provided a method for identifying an anti-mitotic agent comprising providing the atomic coordinates comprising the relative atomic structural coordinates of the amino acids of Figure 10 as set forth in Tables 1-4 ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 2.00Å thereof to a computerized modeling system; modeling compounds which fit spacially into the KSP binding site; and identifying in an assay for KSP activity a compound that inhibits or decreases the activity of the KSP through binding to the binding site.

Once the agent has been identified, it may be contacted with KSP and the effect the agent has on KSP may then be assessed. In addition, the agent may be contacted with KSP in the presence of a KSP binding molecule and the effect the agent has on binding between KSP and the KSP binding molecule may then be assessed.

Also disclosed herein is a process for identifying a potential anti-mitotic agent which upon binding to a human KSP inhibits cell proliferation, the process comprising the steps of:

- exposing the KSP to a mixture of at least two potential ligands;
- attempting to crystallize said KSP in the presence of said mixture;
- c) if crystals are obtained, obtaining an X-ray diffraction pattern of the KSP crystal; and
- d) determining whether a ligand/KSP complex is formed by comparing the electron density map calculated from the X-ray diffraction pattern of said KSP crystal

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when exposed to said mixture of said at least two potential ligands to the electron density map calculated from the X-ray diffraction pattern set forth in a table selected from Table 1, 2, 3 and 4.

Also provided herein is a method of identifying a compound that modulates the binding of a ligand to a ligand binding site of a human KSP, said method comprising: modeling test compounds that fit spatially into a KSP ligand binding site using an atomic structural model of a KSP binding site having the relative structural coordinates as set forth in a table selected from the group consisting of Tables 1, 2, 3 and 4 for the KSP amino acid residues 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F), ± the root mean square deviation from

the backbone atoms of said amino acids of not more than about 2.0 Å;
screening the test compounds in an assay characterized by binding of a ligand to the ligand binding site; and identifying a test compound that modulates binding of said ligand to the KSP at its binding site.

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Further provided is a method for identifying a potential inhibitor of human kinesin spindle protein (KSP), the method comprising the steps of :

- (i) providing a three-dimensional structure of a ligandbound KSP as defined by atomic coordinates set forth in a table selected from Tables 1, 2, 3 and 4;
- (ii) comparing the three-dimensional coordinates of the
 25 ligand when it is bound to KSP as set forth in Table 1, 2, 3 or 4 to the three-dimensional coordinates of a compound in a database of compound structures; and
 - (iii) selecting from said database at least one compound that is structurally similar to said ligand when it is bound to said KSP, wherein the selected compound is a potential inhibitor of said KSP.

Also provided is a method for identifying an anti-mitotic agent which upon binding to a target human KSP inhibits cell proliferation, the method comprising the steps of:

a) exposing a target KSP to a mixture of at least two potential ligands;

b) attempting to crystallize said target KSP in the presence of said mixture;

- obtaining a crystal of said target KSP exposed to said mixture to determine whether ligand/KSP complex is formed; and
- d) identifying a potential anti-mitotic agent as one that binds to said KSP at a ligand binding site having the relative structural coordinates as set forth in Table 5 ± the root mean square deviation of not more than about 2.0 Å.

Further provided is a method for identifying an anti-mitotic
agent which upon binding to a target human KSP inhibits cell proliferation,
the method comprising the steps of:

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- (a) obtaining a crystal of KSP, where said KSP has been crystallized while exposed to a mixture of at least two potential ligands;
- (b) determining whether a ligand/KSP complex is formed in said crystal; and
 - (c) identifying a potential anti-mitotic agent as one that binds to said KSP at a ligand binding site having the relative structural coordinates as set forth in Table 5 ± the root mean square deviation of not more than about 2.0 Å.
- In the methods described hereinabove, potential ligands of KSP include the test compounds and Mg++ and ADP.

Also provided is a method of modulating, e.g., inhibiting the activity of a KSP. The method can be *in vitro* or *in vivo*. The method comprises administering, *in vitro* or *in vivo*, a sufficient amount of a compound that binds to the binding site disclosed herein.

Also provided is a method of identifying a compound that selectively inhibits the activity of one type of KSP compared to other KSPs or kinesins, e.g., a KSP of one species over another or a KSP over another member of the BimC family, of which KSP is a member. Thus, the method enables the identification of KSP and KSP like proteins in the same family, e.g., BimC or the KSP in one species over another. The method is exemplified by modeling test compounds that fit spacially and preferentially into a KSP ligand binding site of interest using an atomic structural model of

a KSP ligand binding site, selecting a compound that interacts with one or more residues of the ligand binding site unique in the context of that site, and identifying in an assay for ligand binding activity a compound that selectively binds to the ligand binding site compared to other KSP. The unique features involved in receptor-selective ligand binding can be identified by comparing atomic models of different receptors or isoforms of the same type of receptor.

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The present invention also provides for computer programs for the expression (such as visual display) of the KSP or analog three-dimensional structure, and further, a computer program which expresses the identity of each constituent of a KSP molecule and the precise location within the overall structure of that constituent, down to the atomic level.

There are many currently available computer programs for the expression of the three-dimensional structure of a molecule. Generally, these programs provide for inputting of the coordinates for the three-dimensional structure of a molecule (i.e., for example, a numerical assignment for each atom of a KSP molecule along an x, y, and z axis or the assignment for each atom of the binding site described in Tables 1-4), means to express (such as visually display) such coordinates, means to alter such coordinates and means to express an image of a molecule having such altered coordinates. One may program crystallographic information, i.e., the coordinates of the location of the atoms of a KSP binding site molecule in three dimension space, wherein such coordinates have been obtained from crystallographic analysis of said KSP molecule, into such programs to generate a computer program for the expression (such as visual display) of the KSP three-dimensional structure.

In furtherance of the above, the present invention provides a machine, such as a computer, programmed in memory with the coordinates of KSP or portions thereof, together with a program capable of converting the coordinates into a three-dimensional graphical representation of the structural coordinates on a display connected to the machine.

As well, there is provided a computer program for the expression of KSP's three-dimensional structure together with the structure of the novel KSP binding site. Preferred is the computer program QUANTA 2000, available from Molecular simulations or Insight II, version 4, available

from Biosym, San Diego, Calif., with the coordinates of the amino acids of Figure 10 as set forth in Tables 1-4 input. Preferred expression means are well known to a skilled artisan. Alternatively, the present KSP crystallographic coordinates and diffraction data are also deposited in the Protein Data Bank, Chemistry Department, Brookhaven National Laboratory, Upton, N.Y. 119723, USA. One may use these data in preparing a different computer program for expression of the three-dimensional structure of a KSP molecule or analog thereof.

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Structural coordinates of a crystalline composition of this invention may be stored in a machine-readable form on a machine-readable storage medium, e.g. a computer hard drive, diskette, DAT tape, etc., for display as a three-dimensional shape or for other uses involving computer-assisted manipulation of, or computation based on, the structural coordinates or the three-dimensional structures they define. For example, data defining the three-dimensional structure of a KSP protein or portions or structurally similar homologues of such proteins, may be stored in a machine-readable storage medium, and may be displayed as a graphical three-dimensional representation of the protein structure, typically using a computer capable of reading the data from said storage medium and programmed with instructions for creating the representation from such data.

This invention thus encompasses a machine, such as a computer, having a memory which contains data representing the structural coordinates of a crystalline composition of this invention, e.g. the coordinates set forth in Tables 1-4, together with additional optional data and instructions for manipulating such data. Such data may be used for a variety of purposes, such as the elucidation of other related structures and drug discovery. For example, a machine having a memory containing such data aids in the rational design or selection of inhibitors of KSP binding or activity, including the evaluation of the ability of a particular chemical entity to favorably associate with KSP as disclosed herein, as well as in the modeling of compounds, proteins, complexes, etc. related by structural or sequence homology to KSP.

Thus, three-dimensional modeling of KSP provided by the present invention using the coordinates from the X-ray diffraction patterns can be entered into one or more computer programs for molecular modeling.

Such molecular modeling programs generate atomic coordinates that reflect the secondary, tertiary and/or quaternary structures of the protein which contribute to its overall three-dimensional structure and provide information related to binding and/or active sites of the protein.

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The present invention further contemplates the use of the structural coordinates of the present invention with standard homology modeling techniques to determine the unknown three-dimensional structure of a target molecule or molecular complex. Homology modeling involves constructing a model of an unknown structure using structural coordinates of one or more related protein molecules/molecular complexes or parts thereof (i.e., ligand binding sites). In general, homology modeling entails fitting. common or homologous portions of the protein whose three-dimensional structure is to be solved to the three-dimensional structure of homologous structural elements in the known molecule, specifically using the relevant (i.e., homologous) structural coordinates provided in Tables 1-4. Homology may be determined using amino acid sequence identity, homologous secondary structure elements, and/or homologous tertiary folds. Homology modeling can include rebuilding part or all of a three-dimensional structure with replacement of amino acids (or other components) by those of the related structure to be solved. Examples of programs for homology modeling include, but are not limited to: QUANTA (Molecular Simulations, Inc.), Molecular Operating Environment or MOE (Chemical Computing Group, Inc. 2002), MODELLER (copyright @ 1989-2002 Andrej Sali; Departments of Biopharmaceutical Sciences and Pharmaceutical Chemistry, and California Institute for Quantitative Biomedical Research, Mission Bay Genentech Hall, University of California San Francisco) and others.

In accordance with the above, a three-dimensional structure for the unknown molecule/molecular complex may be generated using the three-dimensional structure of the KSP molecule of the present invention, Tables 1-4, refined using a number of techniques well known in the art, and then used in the same fashion as the structural coordinates of the present invention, for instance, in applications involving molecular replacement analysis, homology modeling, and rational drug design.

Among other aspects, the coordinates in Table 1-4 define the relative relationship between the protein, the nucleotide and the ligand. Such sets of

coordinates are dependent upon the particular coordinate system used. Those skilled in the art will recognize that rotation, translation or other mathematical manipulation of these coordinates may change the specific values of these coordinates, but the new set(s) will still define the relationship between the multiple components of the crystal structure disclosed herein."

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The determination of the three-dimensional structure of the ligand binding site of KSP as disclosed herein is advantageous over conventional drug assay techniques, in which the only way to identify such an agent is to screen thousands of test compounds until an agent having the desired inhibitory effect on a target compound is identified. Generally, such conventional screening methods are expensive, time consuming, and do not elucidate the method of action of the identified agent on the target compound. In sharp contrast, advancing X-ray, spectroscopic and computer modeling technologies allow researchers to visualize the three-dimensional structure of a targeted compound (i.e., KSP ligand binding site), and using such a three-dimensional structure to identify putative binding sites and then identify or design agents to interact with these binding sites. These agents can thereafter be screened for an inhibitory effect upon the target molecule. Consequently, an embodiment of the invention details a method for identifying a potential inhibitor of KSP. The proposed method comprises using a three-dimensional structure of KSP and the novel binding site of the invention as defined by the relative structural coordinates of Tables 1-4 and the relative structural coordinates of the amino acid residues of Figure 10 as set forth in Table 1-4 to design or select a potential inhibitor of KSP activity, followed by synthesizing or obtaining the said potential inhibitor. The inhibitor may be selected by screening an appropriate database. Alternatively, it may be designed de novo by analyzing the steric configurations and charge potentials of a ligand bound KSP complex in conjunction with the appropriate software programs, or may be designed using characteristics of known inhibitors of KSP.

An entity/agent that interacts or associates with the ligand binding site of KSP may be identified by performing computer fitting analyses to identify an agent which interacts or associates with said site. Computer fitting analyses utilize various computer software programs that evaluate the "fit" between the binding site and the identified agent, by (a)

generating a three-dimensional model of the ligand binding site using homology modeling or the atomic structural coordinates of the binding site in Tables 1-4, and (b) determining the degree of association between the binding site and the identified agent. The degree of association may be determined computationally by any number of commercially available software programs, or may be determined experimentally using standard binding assays.

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Preferably, the method of the present invention includes the use of a ligand binding site characterized by the three-dimensional structure comprising the relative structural coordinates of amino acid residues listed in Figure 10 as set forth in Tables 1-4 ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 2.0 Å, preferably not more than about 1.0 Å, and most preferably not more than about 0.5 Å. It is understood that the method of the present invention includes additional embodiments comprising conservative substitutions of the noted amino acids which result in the same structural coordinates of the corresponding residues in Tables 1-4 within the stated root mean square deviation.

The effect of an agent identified by computer fitting analyses on human KSP activity may be further evaluated computationally, or experimentally by competitive binding experiments or by contacting the identified agent with KSP and measuring the effect of the agent on the target's biological activity. Standard enzymatic assays may be performed and the results analyzed to determine whether the agent is an inhibitor of KSP activity (i.e., induce cell cycle arrest or inhibit the association of KSP with a microtubule as well as any other known activities attending a kinesin). Further tests may be performed to evaluate the selectivity of the identified agent to KSP with regard to other KSP proteins (other species) or other members of the BimC protein family.

Preferably, the agent designed or selected to interact with KSP is capable of associating with KSP and of assuming a three-dimensional configuration and orientation that complements the relevant ligand binding site of KSP.

Consequently, using these criteria, the structural coordinates of the KSP molecule as disclosed herein, and/or structural coordinates

derived therefrom using molecular replacement or homology modeling, agents may be designed having increased potency and/or selectivity versus known inhibitors, e.g, by modifying the structure of known inhibitors or by designing new agents de novo via computational inspection of the three-dimensional configuration of KSP's novel ligand binding site described herein (relative structural coordinates of amino acid residues listed in Figure 10 as set forth in Tables 1-4 and the relative structural coordinates set forth in Table 5).

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As such, an embodiment of the invention proposes using the structural coordinates of Tables 1-4 of the present invention, or structural coordinates derived therefrom using molecular replacement or homology modeling techniques as discussed above to screen a database for agents that may act as potential inhibitors of KSP activity. As an example, the obtained structural coordinates of the present invention may be read into a software package and the three-dimensional structure analyzed graphically. A number of computational software packages may be used for the analysis of structural coordinates, e.g., Sybyl (Tripos Associates) etc. Additional software programs may be optionally used to check the coordinates with regard to features such as bond and atom types. If necessary, the threedimensional structure may be modified and then energy minimized using the appropriate software until all of the structural parameters are at their equilibrium/optimal values. The energy minimized structure can then be superimposed against the original structure to make sure there are no significant deviations between the original and the energy minimized coordinates.

Once the specific interaction between KSP and a known inhibitor is determined, e.g., such as the information provided in Tables 1-4, docking studies with different inhibitors will allow one skilled in the art to generate initial models of new inhibitors bound to KSP. The integrity of these new models may be evaluated a number of ways, including constrained conformational analysis using molecular dynamics methods; that is where both KSP and the bound inhibitor are allowed to sample different three-dimensional conformational states until the most favorable state is reached or found to exist between the protein and the bound agent etc. Once models are obtained of the original known agent bound to KSP

(Tables 1-4) and computer models of other molecules bound to KSP are as well obtained, strategies may be proposed determined for designing modifications into the inhibitors to improve their activity and/or enhance their selectivity.

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For example, once a KSP binding agent has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or side groups in order to improve or modify its selectivity and binding properties for KSP. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. Such substituted chemical compounds may then be analyzed for efficiency of fit to KSP by the same computer methods described in detail above. Further molecular analysis and rational drug design techniques are disclosed in U.S. Pat. Nos. 5,834,228, and 5,939,528 the contents of which are incorporated by reference in their entirety.

Thus, an exemplary embodiment of the invention envisions a method of three-dimensional modeling of a KSP protein, comprising the steps of:

- (a) providing three-dimensional atomic coordinates derived from
 X-ray diffraction measurements of a KSP protein in a computer readable format;
 - (b) inputting the data from step (a) into a computer with appropriate software programs; and
- (c) generating a three-dimensional structural representation of the KSP protein suitable for visualization and further computational manipulation.

This invention further provides for the use of the structural coordinates of a crystalline composition of this invention, or portions thereof, to identify reactive amino acids within the three-dimensional structure, preferably within or adjacent to a ligand binding site; to generate and visualize a molecular surface, such as a water-accessible surface or a surface comprising the space-filling van der Waals surface of all atoms; to calculate and visualize the size and shape of surface features of the protein or complex, e.g., ligand binding pockets; to locate potential H-bond donors and acceptors within the three-dimensional structure, preferably within or

adjacent to a ligand binding site; to calculate regions of hydrophobicity and hydrophilicity within the three-dimensional structure, preferably within or adjacent to a ligand binding site; and to calculate and visualize regions on or adjacent to the protein surface of favorable interaction energies with respect to selected functional groups of interest (e.g. amino, hydroxyl, carboxyl, methylene, alkyl, alkenyl, aromatic carbon, aromatic rings, heteroaromatic rings, substituted and unsubstituted phosphates, substituted and unsubstituted phosphonates, substituted and unsubstituted fluoro and difluorophosphonates; etc.). One may use the foregoing approaches for characterizing the protein and its interactions with moieties of potential ligands to design or select compounds capable of specific covalent attachment to reactive amino acids (e.g., cysteine) and to design or select compounds of complementary characteristics (e.g., size, shape, charge, hydrophobicity/hydrophilicity, ability to participate in hydrogen bonding, etc.) to surface features of the protein, a set of which may be preselected. Using the structural coordinates, one may also predict or calculate the orientation, binding constant or relative affinity of a given ligand to the protein in the complexed state, and use that information to design or select compounds of improved affinity.

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In such cases, the structural coordinates of the KSP protein, or portion or complex thereof, are entered in machine readable form into a machine programmed with instructions for carrying out the desired operation and containing any necessary additional data, e.g. data defining structural and/or functional characteristics of a potential ligand or moiety thereof, defining molecular characteristics of the various amino acids, etc.

The present invention is additionally directed to a method of determining the three-dimensional structure of a molecule or molecular complex whose structure is unknown, comprising the steps of first obtaining crystals of the molecule or molecular complex whose structure is unknown, and then generating X-ray diffraction data from the crystallized molecule or molecular complex and/or generating NMR data from the solution of the molecule or molecular complex. The generated diffraction or spectroscopy data from the molecule or molecular complex can then be compared with the solution coordinates or three-dimensional structure of KSP as disclosed herein, and the three-dimensional structure of the unknown molecule or

molecular complex conformed to the KSP structure using standard techniques such as molecular replacement analysis, 2D, 3D and 4D isotope filtering, editing and triple resonance NMR techniques, and computer homology modeling. Alternatively, a three-dimensional model of the unknown molecule may be generated by generating a sequence alignment between KSP and the unknown molecule, based on any or all of amino acid sequence identity, secondary structure elements or tertiary folds, and then generating by computer modeling a three-dimensional structure for the molecule using the three-dimensional structure of, and sequence alignment with, KSP.

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Preferred embodiments of the aforementioned methods are those methods wherein the KSP protein comprises a binding site characterized by amino acid residues described in Figure 10.

This invention also provides peptidomimetic methods for designing a compound capable of binding to a KSP protein or KSP homolog. One such method involves graphically displaying a three-dimensional representation based on coordinates defining the three-dimensional structure of a KSP family protein or a portion thereof complexed with a ligand. Interactions between portions of a ligand and the protein may then be analyzed in order to identify candidate moieties for replacement. One or more portions of the ligand which interact with the protein may be replaced with substitute moieties selected from a knowledge base of one or more candidate substitute moieties, and/or moieties may be added to the ligand to permit additional interactions with the protein.

In another aspect of the instant invention, the structural coordinates of a crystalline composition of this invention, or portions thereof, may be used to identify one or more pharmacophores of a chemical compound that binds to the ligand binding site. Such a pharmacophore is described as a set of atoms, chemical groups, pseudo-atoms or vectors, and the relative positions in space of each of these pharmacophore features. Each feature, alone or in combination with its relative position, forms a pharmacophore parameter. Thus, the pharmacophore includes the pharmacophore features, and the relative position of each descriptor with regard to all other descriptors comprising the pharmacophore.

Pharmacophore models can be constructed either directly or indirectly. In the direct method, the pharmacophore feature spatial centers are inferred from

studying the X-ray structural coordinates or NMR structure of a receptor-ligand complex, followed by a shape-complementarity function analysis of the receptor binding site, usually performed using a computer and a computer-readable medium. In the indirect method, the structure of the receptor is unknown and the pharmacophore feature spatial centers are inferred by overlaying the three-dimensional conformations of active compounds and finding the common, overlapping functional groups.

The pharmacophore models of the present invention, obtained by combining both direct and indirect methods, are herein described, by way of example only and without any intention of being limiting, with reference to Figures 14A and B.

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The first model pharmacophore (FIG. 14A) is represented by three pharmacophore features having the planar orientation shown: a sphere indicating the center of an aryl, heteroaryl or cycloalkyl ring (or, in general, of a hydrophobic group), and two small boxes (labeled HA and HD), representing the heterocenters of a hydrogen bond acceptor and a hydrogen bond donor, respectively. The second model pharmacophore (FIG. 14B) is represented by three pharmacophore features: two spheres indicating the centers of two aryl, heteroaryl or cycloalkyl rings (or hydrophobic groups in general), and a small box representing the heteroatomic center of a hydrogen bond acceptor (HA).

As used herein, "aryl" is intended to mean any stable monocyclic or bicyclic carbon ring of up to 7 atoms in each ring, wherein at least one ring is aromatic. Examples of such aryl elements include phenyl, naphthyl, tetrahydronaphthyl, indanyl and biphenyl. In cases where the aryl substituent is bicyclic and one ring is non-aromatic, it is understood that attachment is via the aromatic ring.

The term heteroaryl, as used herein, represents a stable monocyclic or bicyclic ring of up to 7 atoms in each ring, wherein at least one ring is aromatic and contains from 1 to 4 heteroatoms selected from the group consisting of O, N and S. Heteroaryl groups within the scope of this definition include but are not limited to: acridinyl, carbazolyl, cinnolinyl, quinoxalinyl, pyrrazolyl, indolyl, benzotriazolyl, furanyl, thienyl, benzothienyl, benzofuranyl, quinolinyl, isoquinolinyl, oxazolyl, isoxazolyl, indolyl, pyrazinyl, pyridazinyl, pyridinyl, pyrimidinyl, pyrrolyl, tetrahydroquinoline. In an embodiment of the instant invention, heteroaryl does not include quinazolinone.

As used herein, "cycloalkyl" is intended to include monocyclic saturated aliphatic hydrocarbon groups having the specified number of carbon atoms.

For example, "cycloalkyl" includes cyclopropyl, methyl-cyclopropyl, 2,2-dimethyl-cyclobutyl, 2-ethyl-cyclopentyl, cyclohexyl, and so on. In an embodiment of the invention the term "cycloalkyl" includes the groups described immediately above and further includes monocyclic unsaturated aliphatic hydrocarbon groups. For example, "cycloalkyl" as defined in this embodiment includes cyclopropyl, methyl-cyclopropyl, 2,2-dimethyl-cyclobutyl, 2-ethyl-cyclopentyl, cyclohexyl, cyclopentenyl, cyclobutenyl and so on.

The, cycloalkyl, aryl, heteroaryl and heteroaryl substituents may be substituted or unsubstituted, unless specifically defined otherwise. For example, an aryl may be substituted with one, two or three substituents selected from OH, alkyl, halogen, alkoxy or dialkylamino.

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The active structural motifs designated herein as the model pharmacophores of the present invention can be used to screen libraries of molecules for the existence of a predefined structural motif, and in particular identifying molecules that meet the constraints imposed by the pharmacophore. The pharmacophore feature spatial centers are globally associated with a specific biological activity. The molecules being evaluated may be designed *de novo* using computer methods, or alternatively, be either a scaffold or a full chemical entity (e.g., chosen from a library of compounds). Using the model pharmacophores disclosed herein one of ordinary skill may predict the inhibitory potency of a compound based upon its fit with any of these two pharmacophore models shown in FIG. 14A and B.

In an embodiment, the compound identified by the use of a pharmacophore model described herein has a binding affinity for KSP of about 0.1 nM to about 100 nM. In a further embodiment, the binding affinity range is from about 1 nM to about 20 nM.

In an embodiment, the compound identified by its fit with the pharmacophore model of Figure 14A does not incorporate a 2-thioxo-1,2,3,4-tetrahydropyrimidine moiety, a dihydropyrimidine moiety or a 5,6,11,11a-tetrahydro-1H-imidazo[1',5':1,6]-pyrido[3.4-b]indole-1,3(2H)-dione moiety.

An additional pharmacophore model is illustrated by Figure 16. The pharmacophore model of Figure 16 is represented by four pharmacophore features: three spheres indicating the centers of aryl, heteroaryl or cycloalkyl rings (or hydrophobic groups in general), and a small box representing the heteroatomic center of a hydrogen bond acceptor (HA). In reference to Figure 16, the distances in Å between the pharmacophore features are listed in the following table:

	1	2	3	4
1	-			
2	5.1±0.6	-		
3	8.5±0.7	6.9±0.7	-	
4	3.7±0.5	5.8±0.6	5.7±0.7	•

In an embodiment, the compound identified by its fit with the pharmacophore model of Figure 16 does not incorporate a quinazolinone, phenothiazine, thienopyrimidinone, furanopyrimidinone, azolopyrimidinone, thiazolopyrimidine, cycloalkylpyrimidinone or triphenylmethane moiety. In a further embodiment, the compound identified by its fit with the pharmacophore model of Figure 16 does not incorporate a quinazolinone, phenothiazine or triphenylmethane moiety.

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In an embodiment, the compound identified by its fit with the pharmacophore model of Figure 14B does not incorporate a quinazolinone, phenothiazine, thienopyrimidinone, furanopyrimidinone, azolopyrimidinone, thiazolopyrimidine, cycloalkylpyrimidinone or triphenylmethane moiety. In a further embodiment, the compound identified by its fit with the pharmacophore model of Fig. 14B does not incorporate a quinazolinone, phenothiazine or triphenylmethane moiety.

The degree of fit of a particular compound structure to the pharmacophore models is calculated by determining, using computer methods, if the compound possesses the chemical features of the pharmacophore model and if the features can adopt the necessary three-dimensional arrangement to fit the model. The modeling program will indicate those features in the pharmacophore model having a fit with the particular compound or chemical feature of the compound being tested. The term "fit" when referring to a compound and a pharmacophore or binding site includes both compounds that occupy only the spatial area of the pharmacophore or binding site and compounds of which the chemical features or a portion of the molecule occupy the spatial area of the pharmacophore or binding site.

Fitting of a compound to the ligand binding site volume can be done in a number of different ways using computational methods well known by those skilled in the art. Visual inspection and manual docking of compounds into the induced-fit active site volume can be done using molecular modeling software such as QUANTA (Molecular Simulations, Burlington, MA, 1992), SYBYL (Tripos Associates, Inc., St. Louis, MO, 1992), AMBER (Weiner et al., J. Am. Chem. Soc., 106: 765-784, 1984), CHARMM (Brooks et al., J. Comp. Chem., 4: 187-217, 1983) or other modeling

programs known to those of skill in the art. This modeling step may be followed by energy minimization using standard force fields, such as CHARMM and AMBER, or others. More specialized modeling programs include MCSS (Miranker & Karplus, Function and Genetics, 11: 29-34, 1991), GRID (Goodford et al., J. Med. Chem., 28: 849-857, 1985), AUTODOCK (Goodsell & Olsen, Proteins: Structure, Function and Genetics, 8: 195-202, 1990), and DOCK (Kuntz et al., J. Mol. Biol., 161: 269-288, 1982). In addition, inhibitor compounds may be constructed *de novo* in the empty active site or in the active site including some portions of a known inhibitor using computer programs such as LEGEND (Nishibata & Itai, Tetrahedron, 47: 8985, 1991), LeapFrog (Tripos Associates, St. Louis, MO), LUDI (Bohm, J. Comp. Aid. Molec. Design, 6: 61-78, 1992), AutoLudi (Accelrys Inc., San Diego, CA) or others.

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Another aspect of the invention relates to a complementary protein having a structure substantially complementary to the three-dimensional structure according to Tables 1-4; or to a medicinally effective part thereof, particularly a ligand binding region. A complementary protein is one whose three-dimensional structure is substantially complementary to the Tables 1-4 structure or a part thereof, such that the complementary structure may bind thereto and may form a complex. The lifetime of the complex may be long in the case of an inhibiting complementary protein. Of course, binding will also require an appropriate choice of amino acid sequence. Such a complementary protein may act as an inhibitor of KSP. Such inhibitors may be used *in vivo* or *in vitro* to modify the activity of KSP.

In the pharmaceutical industry, new or known compounds are routinely screened for new uses employing a variety of known in vitro or in vivo screens. Often such screens involve complex natural substances and are correspondingly expensive to carry out, and the result may be difficult to interpret. The knowledge of the three-dimensional protein structure according to the invention allows a preliminary screening to be carried out on the basis of the three-dimensional structure of a region thereof, and the structural similarity of a molecule which is being screened. This is usually carried out in conjunction with a knowledge of the amino sequence of the region. Such screening can conveniently be carried out using computer modeling techniques, which match the three-dimensional structure of the protein or part thereof (or complementary protein or part thereof) with the

structure of the molecule being screened, thereby allowing one to predict potential inhibitor activity.

The binding of a ligand to the novel binding site of the instant invention and the formation of the novel binding pocket as a result can also be indirectly assessed by spectroscopically determining the shift in the fluorescence of the amino acid 127 tryptophan residue. Thus it has been discovered that the fluorescent emission of Trp127 is modulated when KSP is treated with one of the inhibitors described above in the presence of a nucleotide or nucleotides.

A further embodiment of the instant invention is an *in vitro* assay for the determination of binding of a test compound to the novel KSP binding site described herein. The assay comprises the steps of:

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- contacting KSP with the test compound and a nucleotide and measuring the fluorescence of the mixture at the peak emission wavelength for Trp127 in KSP;
- contacting KSP with a nucleotide and measuring the fluorescence of the mixture at the peak emission wavelength for Trp127 in KSP; and
- comparing the fluorescence of the mixture of KSP, the test compound and the nucleotide with the fluorescence of the mixture of KSP with the nucleotide alone.

In another embodiment of the *in vitro* fluorescence assay the nucleotide is selected from ADP and AMPPNP (a non-hydrolysable analog of ATP, adenosine 5'- $(\beta,\gamma$ -imido)triphosphate tetralithium salt hydrate).

In an embodiment of the *in vitro* fluorescence assay the mixtures additionally contain a source of magnesium ion. Preferably the source of magnesium ion is MgCl₂.

In another embodiment of the *in vitro* fluorescence assay the measurement of the fluorescence of the KSP, test compound and nucleotide mixture is performed at several different concentrations of the test compound.

Because the KSP kinesin's three-dimensional structure is uniquely suited to the formation of the novel binding pocket of the instant invention, the methods of identification of compounds that bind to the novel binding pocket described herein, such as the fluorescence assay described

above, may be used to identify selective inhibitors of KSP which may not inhibit other mitotic kinesins. Such identification of a selective KSP inhibitor may offer particular advantages over an inhibitor which is competitive with the binding of the nucleotide substrate of KSP or which binds to the site of microtubule binding.

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A still further aspect of the invention relates to antibodies (including monoclonal antibodies) directed to the KSP protein or complementary protein, for the detection thereof or for the modulation of its medicinal activity, it being understood that the antibody is specific for the KSP-ligand, e.g., inhibitor bound conformation.

Compounds of the structures selected or designed by any of the foregoing means may be tested for their ability to bind to a KSP protein, inhibit the binding of a KSP protein to a natural or non-natural ligand therefor, and/or inhibit a biological function mediated by a KSP protein or a BimC family member.

Finally, the present invention provides agents or inhibitors designed or selected using the methods disclosed herein. Such compounds may be utilized as described in the following sections.

Utilities

The compounds designed or selected using the methods of the invention find use in a variety of applications. As will be appreciated by those in the art, mitosis may be altered in a variety of ways; that is, one can affect mitosis either by increasing or decreasing the activity of a component in the mitotic pathway. Stated differently, mitosis may be affected (e.g., disrupted) by disturbing equilibrium, either by inhibiting or activating certain components. Similar approaches may be used to alter meiosis.

In a preferred embodiment, the compounds designed or selected using the methods of the invention are used to modulate mitotic spindle formation, thus causing prolonged cell cycle arrest in mitosis. By "modulate" herein is meant altering mitotic spindle formation, including increasing and decreasing spindle formation. By "mitotic spindle formation" herein is meant organization of microtubules into bipolar structures by mitotic kinesins. By "mitotic spindle dysfunction" herein is meant mitotic arrest and monopolar spindle formation.

The compounds designed or selected using the methods of the invention are useful to bind to and/or modulate the activity of a mitotic kinesin. In a

preferred embodiment, the mitotic kinesin is a member of the bimC subfamily of mitotic kinesins (as described in U.S. Patent No. 6,284,480, column 5). In a further preferred embodiment, the mitotic kinesin is human KSP, although the activity of mitotic kinesins from other organisms may also be modulated by the compounds of the present invention. In this context, modulate means either increasing or decreasing spindle pole separation, causing malformation, i.e., splaying, of mitotic spindle poles, or otherwise causing morphological perturbation of the mitotic spindle. Also included within the definition of KSP for these purposes are variants and/or fragments of KSP. See PCT Publ. WO 01/31335: "Methods of Screening for Modulators of Cell Proliferation and Methods of Diagnosing Cell Proliferation States", filed Oct. 27, 1999, hereby incorporated by reference in its entirety. In addition, other mitotic kinesins may be inhibited by the compounds of the present invention.

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The compounds designed or selected using the methods of the invention are used to treat cellular proliferation diseases. Disease states which can be treated by the methods and compositions provided herein include, but are not limited to, cancer (further discussed below), autoimmune disease, arthritis, graft rejection, inflammatory bowel disease, proliferation induced after medical procedures, including, but not limited to, surgery, angioplasty, and the like. It is appreciated that in some cases the cells may not be in a hyper- or hypoproliferation state (abnormal state) and still require treatment. For example, during wound healing, the cells may be proliferating "normally", but proliferation enhancement may be desired. Similarly, as discussed above, in the agriculture arena, cells may be in a "normal" state, but proliferation modulation may be desired to enhance a crop by directly enhancing growth of a crop, or by inhibiting the growth of a plant or organism which adversely affects the crop. Thus, in one embodiment, the invention herein includes application to cells or individuals afflicted or impending affliction with any one of these disorders or states.

The compounds, compositions and methods provided herein are particularly deemed useful for the treatment of cancer including solid tumors such as skin, breast, brain, cervical carcinomas, testicular carcinomas, etc. More particularly, cancers that may be treated by the compounds, compositions and methods of the invention include, but are not limited to: <u>Cardiac</u>: sarcoma (angiosarcoma, fibrosarcoma, rhabdomyosarcoma, liposarcoma), myxoma, rhabdomyoma, fibroma, lipoma and teratoma; Lung: bronchogenic carcinoma (squamous cell, undifferentiated small cell, undifferentiated large cell, adenocarcinoma), alveolar (bronchiolar)

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carcinoma, bronchial adenoma, sarcoma, lymphoma, chondromatous hamartoma, mesothelioma; Gastrointestinal: esophagus (squamous cell carcinoma, adenocarcinoma, leiomyosarcoma, lymphoma), stomach (carcinoma, lymphoma, leiomyosarcoma), pancreas (ductal adenocarcinoma, insulinoma, glucagonoma, gastrinoma, carcinoid tumors, vipoma), small bowel (adenocarcinoma, lymphoma, carcinoid tumors, Karposi's sarcoma, leiomyoma, hemangioma, lipoma, neurofibroma, fibroma), large bowel (adenocarcinoma, tubular adenoma, villous adenoma, hamartoma, leiomyoma); Genitourinary tract: kidney (adenocarcinoma, Wilm's tumor [nephroblastoma], lymphoma, leukemia), bladder and urethra (squamous cell carcinoma, transitional cell carcinoma, adenocarcinoma), prostate (adenocarcinoma, sarcoma), testis (seminoma, teratoma, embryonal carcinoma, teratocarcinoma, choriocarcinoma, sarcoma, interstitial cell carcinoma, fibroma, fibroadenoma, adenomatoid tumors, lipoma); Liver: hepatoma (hepatocellular carcinoma), cholangiocarcinoma, hepatoblastoma, angiosarcoma, hepatocellular adenoma, hemangioma; Bone: osteogenic sarcoma (osteosarcoma), fibrosarcoma, malignant fibrous histiocytoma, chondrosarcoma, Ewing's sarcoma, malignant lymphoma (reticulum cell sarcoma), multiple mycloma, malignant giant cell tumor chordoma, osteochronfroma (osteocartilaginous exostoses), benign chondroma, chondroblastoma, chondromyxofibroma, osteoid osteoma and giant cell tumors; Nervous system: skull (osteoma, hemangioma, granuloma, xanthoma, osteitis deformans), meninges (meningioma, meningiosarcoma, gliomatosis), brain (astrocytoma, medulloblastoma, glioma, ependymoma, germinoma [pinealoma], glioblastoma multiform, oligodendroglioma, schwannoma, retinoblastoma, congenital tumors), spinal cord neurofibroma, meningioma, glioma, sarcoma); Gynecological: uterus (endometrial carcinoma), cervix (cervical carcinoma, pre-tumor cervical dysplasia), ovaries (ovarian carcinoma [serous cystadenocarcinoma, mucinous cystadenocarcinoma, unclassified carcinoma], granulosa-thecal cell tumors, Sertoli-Leydig cell tumors, dysgerminoma, malignant teratoma), vulva (squamous cell carcinoma, intraepithelial carcinoma, adenocarcinoma, fibrosarcoma, melanoma), vagina (clear cell carcinoma, squamous cell carcinoma, botryoid sarcoma (embryonal rhabdomyosarcoma), fallopian tubes (carcinoma); Hematologic: blood (myeloid leukemia [acute and chronic], acute lymphoblastic leukemia, chronic lymphocytic leukemia, myeloproliferative diseases, multiple myeloma, myelodysplastic syndrome). Hodgkin's disease, non-Hodgkin's lymphoma [malignant lymphoma]; Skin: malignant melanoma, basal cell carcinoma, squamous cell carcinoma, Karposi's sarcoma, moles

dysplastic nevi, lipoma, angioma, dermatofibroma, keloids, psoriasis; and <u>Adrenal</u> glands: neuroblastoma. Thus, the term "cancerous cell" as provided herein, includes a cell afflicted by any one of the above-identified conditions.

The compounds designed or selected using the methods of the instant invention may also be useful as antifungal agents, by modulating the activity of the fungal members of the bimC kinesin subgroup, as is described in U.S. Patent No. 6.284,480.

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The compounds designed or selected using the methods of this invention may be administered to mammals, preferably humans, either alone or, preferably, in combination with pharmaceutically acceptable carriers, excipients or diluents, in a pharmaceutical composition, according to standard pharmaceutical practice. The compounds can be administered orally or parenterally, including the intravenous, intramuscular, intraperitoneal, subcutaneous, rectal and topical routes of administration.

As used herein, the term "composition" is intended to encompass a product comprising the specified ingredients in the specific amounts, as well as any product which results, directly or indirectly, from combination of the specific ingredients in the specified amounts.

The pharmaceutical compositions containing the active ingredient may be in a form suitable for oral use, for example, as tablets, troches, lozenges, aqueous or oily suspensions, dispersible powders or granules, emulsions, hard or soft capsules, or syrups or elixirs. Compositions intended for oral use may be prepared according to any method known to the art for the manufacture of pharmaceutical compositions and such compositions may contain one or more agents selected from the group consisting of sweetening agents, flavoring agents, coloring agents and preserving agents in order to provide pharmaceutically elegant and palatable preparations. Tablets contain the active ingredient in admixture with non-toxic pharmaceutically acceptable excipients which are suitable for the manufacture of tablets. These excipients may be for example, inert diluents, such as calcium carbonate, sodium carbonate, lactose, calcium phosphate or sodium phosphate; granulating and disintegrating agents, for example, microcrystalline cellulose, sodium crosscarmellose, com starch, or alginic acid, binding agents, for example starch, gelatin, polyvinyl-pyrrolidone or acacia, and lubricating agents, for example, magnesium stearate, stearic acid or talc. The tablets may be uncoated or they may be coated by known techniques to mask the unpleasant taste of the drug or delay disintegration and absorption in the gastrointestinal tract and

thereby provide a sustained action over a longer period. For example, a water soluble taste masking material such as hydroxypropyl-methylcellulose or hydroxypropylcellulose, or a time delay material such as ethyl cellulose, cellulose acetate buryrate may be employed.

Formulations for oral use may also be presented as hard gelatin capsules wherein the active ingredient is mixed with an inert solid diluent, for example, calcium carbonate, calcium phosphate or kaolin, or as soft gelatin capsules wherein the active ingredient is mixed with water soluble carrier such as polyethyleneglycol or an oil medium, for example peanut oil, liquid paraffin, or olive oil.

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Aqueous suspensions contain the active material in admixture with excipients suitable for the manufacture of aqueous suspensions. Such excipients are suspending agents, for example sodium carboxymethylcellulose, methylcellulose, hydroxypropylmethyl-cellulose, sodium alginate, polyvinyl-pyrrolidone, gum tragacanth and gum acacia; dispersing or wetting agents may be a naturally-occurring. phosphatide, for example lecithin, or condensation products of an alkylene oxide with fatty acids, for example polyoxyethylene stearate, or condensation products of ethylene oxide with long chain aliphatic alcohols, for example heptadecaethyleneoxycetanol, or condensation products of ethylene oxide with partial esters derived from fatty acids and a hexitol such as polyoxyethylene sorbitol monooleate, or condensation products of ethylene oxide with partial esters derived from fatty acids and hexitol anhydrides, for example polyethylene sorbitan monooleate. The aqueous suspensions may also contain one or more preservatives, for example ethyl, or n-propyl p-hydroxybenzoate, one or more coloring agents, one or more flavoring agents, and one or more sweetening agents, such as sucrose, saccharin or aspartame.

Oily suspensions may be formulated by suspending the active ingredient in a vegetable oil, for example arachis oil, olive oil, sesame oil or coconut oil, or in mineral oil such as liquid paraffin. The oily suspensions may contain a thickening agent, for example beeswax, hard paraffin or cetyl alcohol. Sweetening agents such as those set forth above, and flavoring agents may be added to provide a palatable oral preparation. These compositions may be preserved by the addition of an anti-oxidant such as butylated hydroxyanisol or alpha-tocopherol.

Dispersible powders and granules suitable for preparation of an aqueous suspension by the addition of water provide the active ingredient in

admixture with a dispersing or wetting agent, suspending agent and one or more preservatives. Suitable dispersing or wetting agents and suspending agents are exemplified by those already mentioned above. Additional excipients, for example sweetening, flavoring and coloring agents, may also be present. These compositions may be preserved by the addition of an anti-oxidant such as ascorbic acid.

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The pharmaceutical compositions of the invention may also be in the form of an oil-in-water emulsions. The oily phase may be a vegetable oil, for example olive oil or arachis oil, or a mineral oil, for example liquid paraffin or mixtures of these. Suitable emulsifying agents may be naturally occurring phosphatides, for example soy bean lecithin, and esters or partial esters derived from fatty acids and hexitol anhydrides, for example sorbitan monooleate, and condensation products of the said partial esters with ethylene oxide, for example polyoxyethylene sorbitan monooleate. The emulsions may also contain sweetening, flavoring agents, preservatives and antioxidants.

Syrups and elixirs may be formulated with sweetening agents, for example glycerol, propylene glycol, sorbitol or sucrose. Such formulations may also contain a demulcent, a preservative, flavoring and coloring agents and antioxidant.

The pharmaceutical compositions may be in the form of a sterile injectable aqueous solutions. Among the acceptable vehicles and solvents that may be employed are water, Ringer's solution and isotonic sodium chloride solution.

The sterile injectable preparation may also be a sterile injectable oil-inwater microemulsion where the active ingredient is dissolved in the oily phase. For example, the active ingredient may be first dissolved in a mixture of soybean oil and lecithin. The oil solution then introduced into a water and glycerol mixture and processed to form a microemulation.

The injectable solutions or microemulsions may be introduced into a patient's blood stream by local bolus injection. Alternatively, it may be advantageous to administer the solution or microemulsion in such a way as to maintain a constant circulating concentration of the instant compound. In order to maintain such a constant concentration, a continuous intravenous delivery device may be utilized. An example of such a device is the Deltec CADD-PLUSTM model 5400 intravenous pump.

The pharmaceutical compositions may be in the form of a sterile injectable aqueous or oleagenous suspension for intramuscular and subcutaneous administration. This suspension may be formulated according to the known art using

those suitable dispersing or wetting agents and suspending agents which have been mentioned above. The sterile injectable preparation may also be a sterile injectable solution or suspension in a non-toxic parenterally acceptable diluent or solvent, for example as a solution in 1,3-butane diol. In addition, sterile, fixed oils are conventionally employed as a solvent or suspending medium. For this purpose any bland fixed oil may be employed including synthetic mono- or diglycerides. In addition, fatty acids such as oleic acid find use in the preparation of injectables.

Compounds designed or selected using the methods disclosed herein may also be administered in the form of suppositories for rectal administration of the drug. These compositions can be prepared by mixing the drug with a suitable non-irritating excipient which is solid at ordinary temperatures but liquid at the rectal temperature and will therefore melt in the rectum to release the drug. Such materials include cocoa butter, glycerinated gelatin, hydrogenated vegetable oils, mixtures of polyethylene glycols of various molecular weights and fatty acid esters of polyethylene glycol.

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For topical use, creams, ointments, jellies, solutions or suspensions, etc., containing the compound are employed. (For purposes of this application, topical application shall include mouth washes and gargles.)

The compounds designed or selected using the methods of the present invention can be administered in intranasal form via topical use of suitable intranasal vehicles and delivery devices, or via transdermal routes, using those forms of transdermal skin patches well known to those of ordinary skill in the art. To be administered in the form of a transdermal delivery system, the dosage administration will, of course, be continuous rather than intermittent throughout the dosage regimen.

25 Compounds of the present invention may also be delivered as a suppository employing bases such as cocoa butter, glycerinated gelatin, hydrogenated vegetable oils, mixtures of polyethylene glycols of various molecular weights and fatty acid esters of polyethylene glycol.

When a compound according to this invention is administered into a human subject, the daily dosage will normally be determined by the prescribing physician with the dosage generally varying according to the age, weight, sex and response of the individual patient, as well as the severity of the patient's symptoms.

In one exemplary application, a suitable amount of compound is administered to a mammal undergoing treatment for cancer. Administration occurs in an amount between about 0.1 mg/kg of body weight to about 60 mg/kg of body

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weight per day, preferably of between 0.5 mg/kg of body weight to about 40 mg/kg of body weight per day.

The compounds designed or selected using the methods disclosed herein (hereafter referred to as the "instant compounds") are also useful in combination with known therapeutic agents and anti-cancer agents. For example, instant compounds are useful in combination with known anti-cancer agents. Combinations of the presently disclosed compounds with other anti-cancer or chemotherapeutic agents are within the scope of the invention. Examples of such agents can be found in Cancer Principles and Practice of Oncology by V.T. Devita and S. Hellman (editors), 6th edition (February 15, 2001), Lippincott Williams & Wilkins Publishers. A person of ordinary skill in the art would be able to discem which combinations of agents would be useful based on the particular characteristics of the drugs and the cancer involved. Such anti-cancer agents include, but are not limited to, the following: estrogen receptor modulators, androgen receptor modulators, retinoid receptor modulators, cytotoxic/cytostatic agents, antiproliferative agents, prenyl-protein transferase inhibitors, HMG-CoA reductase inhibitors and other angiogenesis inhibitors, inhibitors of cell proliferation and survival signaling, and agents that interfere with cell cycle checkpoints. The instant compounds are particularly useful when co-administered with radiation therapy.

In an embodiment, the instant compounds are also useful in combination with known anti-cancer agents including the following: estrogen receptor modulators, androgen receptor modulators, retinoid receptor modulators, cytotoxic agents, antiproliferative agents, prenyl-protein transferase inhibitors, HMG-CoA reductase inhibitors, HIV protease inhibitors, reverse transcriptase inhibitors, and other angiogenesis inhibitors.

"Estrogen receptor modulators" refers to compounds that interfere with or inhibit the binding of estrogen to the receptor, regardless of mechanism. Examples of estrogen receptor modulators include, but are not limited to, tamoxifen, raloxifene, idoxifene, LY353381, LY117081, toremifene, fulvestrant, 4-[7-(2,2-dimethyl-1-oxopropoxy-4-methyl-2-[4-[2-(1-piperidinyl)ethoxy]phenyl]-2H-1-benzopyran-3-yl]-phenyl-2,2-dimethylpropanoate, 4,4'-dihydroxybenzophenone-2,4-dinitrophenyl-hydrazone, and SH646.

"Androgen receptor modulators" refers to compounds which interfere or inhibit the binding of androgens to the receptor, regardless of mechanism.

Examples of androgen receptor modulators include finasteride and other 5α-reductase inhibitors, nilutamide, flutamide, bicalutamide, liarozole, and abiraterone acetate.

"Retinoid receptor modulators" refers to compounds which interfere or inhibit the binding of retinoids to the receptor, regardless of mechanism. Examples of such retinoid receptor modulators include bexarotene, tretinoin, 13-cis-retinoic acid, 9-cis-retinoic acid, α-difluoromethylomithine, ILX23-7553, trans-N-(4'-hydroxyphenyl) retinamide, and N-4-carboxyphenyl retinamide.

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"Cytotoxic/cytostatic agents" refer to compounds which cause cell death or inhibit cell proliferation primarily by interfering directly with the cell's functioning or inhibit or interfere with cell myosis, including alkylating agents, tumor necrosis factors, intercalators, hypoxia activatable compounds, microtubule inhibitors/microtubule-stabilizing agents, inhibitors of mitotic kinesins, inhibitors of kinases involved in mitotic progression, antimetabolites; biological response modifiers; hormonal/anti-hormonal therapeutic agents, haematopoietic growth factors, monoclonal antibody targeted therapeutic agents, topoisomerase inhibitors, proteosome inhibitors and ubiquitin ligase inhibitors.

Examples of cytotoxic agents include, but are not limited to, sertenef, cachectin, ifosfamide, tasonermin, lonidamine, carboplatin, altretamine, prednimustine, dibromodulcitol, ranimustine, fotemustine, nedaplatin, oxaliplatin, temozolomide, heptaplatin, estramustine, improsulfan tosilate, trofosfamide, nimustine, dibrospidium chloride, pumitepa, lobaplatin, satraplatin, profiromycin, cisplatin, irofulven, dexifosfamide, cis-aminedichloro(2-methyl-pyridine)platinum, benzylguanine, glufosfamide, GPX100, (trans, trans, trans)-bis-mu-(hexane-1,6-diamine)-mu-[diamine-platinum(II)]bis[diamine(chloro)platinum (II)]tetrachloride, diarizidinylspermine, arsenic trioxide, 1-(11-dodecylamino-10-hydroxyundecyl)-3,7-dimethylxanthine, zorubicin, idarubicin, daunorubicin, bisantrene, mitoxantrone, pirarubicin, pinafide, valrubicin, amrubicin, antineoplaston, 3'-deamino-3'-morpholino-13-deoxo-10-hydroxycarminomycin, annamycin, galarubicin, elinafide, MEN10755, and 4-demethoxy-3-deamino-3-aziridinyl-4-methylsulphonyl-daunorubicin (see WO 00/50032).

An example of a hypoxia activatable compound is tirapazamine.

Examples of proteosome inhibitors include but are not limited to lactacystin and MLN-341 (Velcade).

Examples of microtubule inhibitors/microtubule-stabilising agents include paclitaxel, vindesine sulfate, 3',4'-didehydro-4'-deoxy-8'-

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norvincaleukoblastine, docetaxol, rhizoxin, dolastatin, mivobulin isethionate, auristatin, cemadotin, RPR109881, BMS184476, vinflunine, cryptophycin, 2,3,4,5,6pentafluoro-N-(3-fluoro-4-methoxyphenyl) benzene sulfonamide, anhydrovinblastine, N.N-dimethyl-L-valyl-L-valyl-N-methyl-L-valyl-L-prolyl-L-proline-t-butylamide, TDX258, the epothilones (see for example U.S. Pat. Nos. 6,284,781 and 6,288,237)

and BMS188797. In an embodiment the epothilones are not included in the microtubule inhibitors/microtubule-stabilising agents.

Some examples of topoisomerase inhibitors are topotecan, hycaptamine, irinotecan, rubitecan, 6-ethoxypropionyl-3',4'-O-exo-benzylidenechartreusin, 9-methoxy-N,N-dimethyl-5-nitropyrazolo[3,4,5-kl]acridine-2-(6H) propanamine, 1-amino-9-ethyl-5-fluoro-2,3-dihydro-9-hydroxy-4-methyl-1H,12Hbenzo[de]pyrano[3',4':b,7]-indolizino[1,2b]quinoline-10,13(9H,15H)dione, lurtotecan, 7-[2-(N-isopropylamino)ethyl]-(20S)camptothecin, BNP1350, BNP11100. BN80915, BN80942, etoposide phosphate, teniposide, sobuzoxane, 2'-

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dimethylamino-2'-deoxy-etoposide, GL331, N-[2-(dimethylamino)ethyl]-9-hydroxy-15 5,6-dimethyl-6H-pyrido[4,3-b]carbazole-1-carboxamide, asulacrine, (5a, 5aB, 8aa,9b)-9-[2-[N-[2-(dimethylamino)ethyl]-N-methylamino]ethyl]-5-[4-hydro0xy-3,5dimethoxyphenyl]-5,5a,6,8,8a,9-hexohydrofuro(3',4':6,7)naphtho(2,3-d)-1,3-dioxol-6-one, 2,3-(methylenedioxy)-5-methyl-7-hydroxy-8-methoxybenzo[c]-

phenanthridinium, 6,9-bis[(2-aminoethyl)amino]benzo[g]isoguinoline-5,10-dione, 5-20 (3-aminopropylamino)-7,10-dihydroxy-2-(2-hydroxyethylaminomethyl)-6Hpyrazolo[4,5,1-de]acridin-6-one, N-[1-[2(diethylamino)ethylamino]-7-methoxy-9oxo-9H-thioxanthen-4-ylmethyl]formamide, N-(2-(dimethylamino)ethyl)acridine-4carboxamide, 6-[[2-(dimethylamino)ethyl]amino]-3-hydroxy-7H-indeno[2,1-c] 25 quinolin-7-one, and dimesna.

Examples of inhibitors of mitotic kinesins, and in particular the human mitotic kinesin KSP, are described in PCT Publications WO 01/30768 and WO 01/98278, and pending U.S. Ser. Nos. 60/338,779 (filed December 6, 2001), 60/338,344 (filed December 6, 2001), 60/338,383 (filed December 6, 2001), 60/338,380 (filed December 6, 2001), 60/338,379 (filed December 6, 2001) and 60/344,453 (filed November 7, 2001). In an embodiment inhibitors of mitotic kinesins include, but are not limited to inhibitors of KSP, inhibitors of MKLP1, inhibitors of CENP-E, inhibitors of MCAK and inhibitors of Rab6-KIFL.

"Inhibitors of kinases involved in mitotic progression" include, but are not limited to, inhibitors of aurora kinase, inhibitors of Polo-like kinases (PLK) (in particular inhibitors of PLK-1), inhibitors of bub-1 and inhibitors of bub-R1.

"Antiproliferative agents" includes antisense RNA and DNA 5 oligonucleotides such as G3139, ODN698, RVASKRAS, GEM231, and INX3001, and antimetabolites such as enocitabine, carmofur, tegafur, pentostatin, doxifluridine, trimetrexate, fludarabine, capecitabine, galocitabine, cytarabine ocfosfate, fosteabine sodium hydrate, raltitrexed, paltitrexid, emitefur, tiazofurin, decitabine, nolatrexed, pemetrexed, nelzarabine, 2'-deoxy-2'-methylidenecytidine, 2'-fluoromethylene-2'-10 deoxycytidine, N-[5-(2,3-dihydro-benzofuryl)sulfonyl]-N'-(3,4-dichlorophenyl)urea, N6-[4-deoxy-4-[N2-[2(E),4(E)-tetradecadienoyl]glycylamino]-L-glycero-B-L-mannoheptopyranosyl]adenine, aplidine, ecteinascidin, troxacitabine, 4-[2-amino-4-oxo-4,6,7,8-tetrahydro-3H-pyrimidino[5,4-b][1,4]thiazin-6-yl-(S)-ethyl]-2,5-thienoyl-Lglutamic acid, aminopterin, 5-flurouracil, alanosine, 11-acetyl-8-15 (carbamoyloxymethyl)-4-formyl-6-methoxy-14-oxa-1,11-diazatetracyclo(7.4.1.0.0)tetradeca-2,4,6-trien-9-yl acetic acid ester, swainsonine, lometrexol, dexrazoxane, methioninase, 2'-cyano-2'-deoxy-N4-palmitoyl-1-B-D-arabino furanosyl cytosine, 3-

Examples of monoclonal antibody targeted therapeutic agents include those therapeutic agents which have cytotoxic agents or radioisotopes attached to a cancer cell specific or target cell specific monoclonal antibody. Examples include Bexxar.

aminopyridine-2-carboxaldehyde thiosemicarbazone and trastuzumab.

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"HMG-CoA reductase inhibitors" refers to inhibitors of 3-hydroxy-3-methylglutaryl-CoA reductase. Compounds which have inhibitory activity for HMG-CoA reductase can be readily identified by using assays well-known in the art. For example, see the assays described or cited in U.S. Patent 4,231,938 at col. 6, and WO 84/02131 at pp. 30-33. The terms "HMG-CoA reductase inhibitor" and "inhibitor of HMG-CoA reductase" have the same meaning when used herein.

Examples of HMG-CoA reductase inhibitors that may be used include but are not limited to lovastatin (MEVACOR®; see U.S. Patent Nos. 4,231,938, 4,294,926 and 4,319,039), simvastatin (ZOCOR®; see U.S. Patent Nos. 4,444,784, 4,820,850 and 4,916,239), pravastatin (PRAVACHOL®; see U.S. Patent Nos. 4,346,227, 4,537,859, 4,410,629, 5,030,447 and 5,180,589), fluvastatin (LESCOL®; see U.S. Patent Nos. 5,354,772, 4,911,165, 4,929,437, 5,189,164, 5,118,853, 5,290,946 and 5,356,896), atorvastatin (LIPITOR®; see U.S. Patent Nos. 5,273,995,

4,681,893, 5,489,691 and 5,342,952) and cerivastatin (also known as rivastatin and BAYCHOL®; see US Patent No. 5,177,080). The structural formulas of these and additional HMG-CoA reductase inhibitors that may be used in the instant methods are described at page 87 of M. Yalpani, "Cholesterol Lowering Drugs", Chemistry & Industry, pp. 85-89 (5 February 1996) and US Patent Nos. 4,782,084 and 4,885,314. The term HMG-CoA reductase inhibitor as used herein includes all pharmaceutically acceptable lactone and open-acid forms (i.e., where the lactone ring is opened to form the free acid) as well as salt and ester forms of compounds which have HMG-CoA reductase inhibitory activity, and therefor the use of such salts, esters, open-acid and lactone forms is included within the scope of this invention. An illustration of the lactone portion and its corresponding open-acid form is shown below as structures I and II.

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In HMG-CoA reductase inhibitors where an open-acid form can exist, salt and ester forms may be formed from the open-acid, and all such forms are included within the meaning of the term "HMG-CoA reductase inhibitor" as used herein. In an embodiment, the HMG-CoA reductase inhibitor is selected from lovastatin and simvastatin, and in a further embodiment, simvastatin. Herein, the term "pharmaceutically acceptable salts" with respect to the HMG-CoA reductase inhibitor shall mean non-toxic salts of the compounds employed in this invention which are generally prepared by reacting the free acid with a suitable organic or inorganic base, particularly those formed from cations such as sodium, potassium, aluminum, calcium, lithium, magnesium, zinc and tetramethylammonium, as well as those salts formed from amines such as ammonia, ethylenediamine, N-methylglucamine, lysine, arginine, ornithine, choline, N,N'-dibenzylethylenediamine, chloroprocaine, diethanolamine, procaine, N-benzylphenethylamine, 1-p-

chlorobenzyl-2-pyrrolidine-1'-yl-methylbenz-imidazole, diethylamine, piperazine, and tris(hydroxymethyl) aminomethane. Further examples of salt forms of HMG-CoA reductase inhibitors may include, but are not limited to, acetate, benzenesulfonate, benzoate, bicarbonate, bisulfate, bitartrate, borate, bromide, calcium edetate, camsylate, carbonate, chloride, clavulanate, citrate, dihydrochloride, edetate, edisylate, estolate, esylate, fumarate, gluceptate, gluconate, glutamate, glycollylarsanilate, hexylresorcinate, hydrabamine, hydrobromide, hydrochloride, hydroxynapthoate, iodide, isothionate, lactate, lactobionate, laurate, malate, maleate, mandelate, mesylate, methylsulfate, mucate, napsylate, nitrate, oleate, oxalate, pamaote, palmitate, panthothenate, phosphate/diphosphate, polygalacturonate, salicylate, stearate, subacetate, succinate, tannate, tartrate, teoclate, tosylate, triethiodide, and valerate.

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Ester derivatives of the described HMG-CoA reductase inhibitor compounds may act as prodrugs which, when absorbed into the bloodstream of a warm-blooded animal, may cleave in such a manner as to release the drug form and permit the drug to afford improved therapeutic efficacy.

"Prenyl-protein transferase inhibitor" refers to a compound which inhibits any one or any combination of the prenyl-protein transferase enzymes, including farnesyl-protein transferase (FPTase), geranylgeranyl-protein transferase 20 type I (GGPTase-I), and geranylgeranyl-protein transferase type-II (GGPTase-II, also called Rab GGPTase). Examples of prenyl-protein transferase inhibiting compounds include (+)-6-[amino(4-chlorophenyl)(1-methyl-1H-imidazol-5-yl)methyl]-4-(3chlorophenyl)-1-methyl-2(1H)-quinolinone, (-)-6-[amino(4-chlorophenyl)(1-methyl-1H-imidazol-5-yl)methyl]-4-(3-chlorophenyl)-1-methyl-2(1H)-quinolinone, (+)-6-25 [amino(4-chlorophenyl)(1-methyl-1H-imidazol-5-yl) methyl]-4-(3-chlorophenyl)-1methyl-2(1H)-quinolinone, 5(S)-n-butyl-1-(2,3-dimethylphenyl)-4-[1-(4cyanobenzyl)-5-imidazolylmethyl]-2-piperazinone, (S)-1-(3-chlorophenyl) -4-[1-(4cyanobenzyl)-5-imidazolylmethyl]-5-[2-(ethanesulfonyl) methyl)-2-piperazinone, 5(S)-n-Butyl-1-(2-methylphenyl)-4-[1-(4-cyanobenzyl)-5-imidazolylmethyl]-2-30 piperazinone, 1-(3-chlorophenyl) -4-[1-(4-cyanobenzyl)-2-methyl-5imidazolylmethyl]-2-piperazinone, 1-(2,2-diphenylethyl)-3-[N-(1-(4-cyanobenzyl)-1H-imidazol-5-ylethyl)carbamoyl]piperidine, 4-{5-[4-hydroxymethyl-4-(4chloropyridin-2-ylmethyl)-piperidine-1-ylmethyl]-2-methylimidazol-1-ylmethyl) benzonitrile, 4-{5-[4-hydroxymethyl-4-(3-chlorobenzyl)-piperidine-1-ylmethyl]-2-35 methylimidazol-1-ylmethyl}benzonitrile, 4-{3-[4-(2-oxo-2H-pyridin-1-yl)benzyl]-3H-

imidazol-4-ylmethyl} benzonitrile, 4-{3-[4-(5-chloro-2-oxo-2H-[1,2'] bipyridin-5'-ylmethyl]-3H-imidazol-4-ylmethyl} benzonitrile, 4-{3-[4-(2-oxo-2H-[1,2'] bipyridin-5'-ylmethyl]-3H-imidazol-4-ylmethyl} benzonitrile, 4-[3-(2-oxo-1-phenyl-1,2-dihydropyridin-4-ylmethyl)-3H-imidazol-4-ylmethyl} benzonitrile, 18,19-dihydro-19-oxo-5H,17H-6,10:12,16-dimetheno-1H-imidazo[4,3-c][1,11,4] dioxaazacyclononadecine-9-carbonitrile, (±)-19,20-dihydro-19-oxo-5H-18,21-ethano-12,14-etheno-6,10-metheno-22H-benzo[d]imidazo[4,3-k][1,6,9,12] oxatriaza-cyclooctadecine-9-carbonitrile, 19,20-dihydro-19-oxo-5H,17H-18,21-ethano-6,10:12,16-dimetheno-22H-imidazo[3,4-h][1,8,11,14] oxatriazacycloeicosine-9-carbonitrile, and (±)-19,20-dihydro-3-methyl-19-oxo-5H-18,21-ethano-12,14-etheno-6,10-metheno-22H-benzo [d]imidazo[4,3-k][1,6,9,12] oxa-triazacyclooctadecine-9-carbonitrile.

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Other examples of prenyl-protein transferase inhibitors can be found in the following publications and patents: WO 96/30343, WO 97/18813, WO 97/21701, WO 97/23478, WO 97/38665, WO 98/28980, WO 98/29119, WO 95/32987,

U.S. Patent No. 5,420,245, U.S. Patent No. 5,523,430, U.S. Patent No. 5,532,359,
U.S. Patent No. 5,510,510, U.S. Patent No. 5,589,485, U.S. Patent No. 5,602,098,
European Patent Publ. 0 618 221, European Patent Publ. 0 675 112, European Patent
Publ. 0 604 181, European Patent Publ. 0 696 593, WO 94/19357, WO 95/08542, WO 95/11917, WO 95/12612, WO 95/12572, WO 95/10514, U.S. Patent No. 5,661,152,

20 WO 95/10515, WO 95/10516, WO 95/24612, WO 95/34535, WO 95/25086, WO 96/05529, WO 96/06138, WO 96/06193, WO 96/16443, WO 96/21701, WO 96/21456, WO 96/22278, WO 96/24611, WO 96/24612, WO 96/05168, WO 96/05169, WO 96/00736, U.S. Patent No. 5,571,792, WO 96/17861, WO 96/33159, WO 96/34850, WO 96/34851, WO 96/30017, WO 96/30018, WO 96/30362, WO

25 96/30363, WO 96/31111, WO 96/31477, WO 96/31478, WO 96/31501, WO 97/00252, WO 97/03047, WO 97/03050, WO 97/04785, WO 97/02920, WO 97/17070, WO 97/23478, WO 97/26246, WO 97/30053, WO 97/44350, WO 98/02436, and U.S. Patent No. 5,532,359.

For an example of the role of a prenyl-protein transferase inhibitor on angiogenesis see European J. of Cancer, Vol. 35, No. 9, pp. 1394-1401 (1999).

"Angiogenesis inhibitors" refers to compounds that inhibit the formation of new blood vessels, regardless of mechanism. Examples of angiogenesis inhibitors include, but are not limited to, tyrosine kinase inhibitors, such as inhibitors of the tyrosine kinase receptors Flt-1 (VEGFR1) and Flk-1/KDR (VEGFR2),

35 inhibitors of epidermal-derived, fibroblast-derived, or platelet derived growth factors,

MMP (matrix metalloprotease) inhibitors, integrin blockers, interferon-α, interleukin-12, pentosan polysulfate, cyclooxygenase inhibitors, including nonsteroidal anti-inflammatories (NSAIDs) like aspirin and ibuprofen as well as selective cyclooxygenase-2 inhibitors like celecoxib and rofecoxib (PNAS, Vol. 89, p. 7384 (1992); JNCI, Vol. 69, p. 475 (1982); Arch. Opthalmol., Vol. 108, p.573 (1990); Anat. Rec., Vol. 238, p. 68 (1994); FEBS Letters, Vol. 372, p. 83 (1995); Clin, Orthop. Vol. 313, p. 76 (1995); J. Mol. Endocrinol., Vol. 16, p.107 (1996); Jpn. J. Pharmacol., Vol. 75, p. 105 (1997); Cancer Res., Vol. 57, p. 1625 (1997); Cell, Vol. 93, p. 705 (1998); Intl. J. Mol. Med., Vol. 2, p. 715 (1998); J. Biol. Chem., Vol. 274, p. 9116 (1999)), steroidal anti-inflammatories (such as corticosteroids, mineralocorticoids, dexamethasone, prednisone, prednisolone, methylpred, betamethasone), carboxyamidotriazole, combretastatin A-4, squalamine, 6-O-chloroacetyl-carbonyl)-fumagillol, thalidomide, angiostatin, troponin-1, angiotensin II antagonists (see Fernandez et al., J. Lab. Clin. Med. 105:141-145 (1985)), and antibodies to VEGF

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Other therapeutic agents that modulate or inhibit angiogenesis and may also be used in combination with the compounds of the instant invention include agents that modulate or inhibit the coagulation and fibrinolysis systems (see review in Clin. Chem. La. Med. 38:679-692 (2000)). Examples of such agents that modulate or inhibit the coagulation and fibrinolysis pathways include, but are not limited to, heparin (see Thromb. Haemost. 80:10-23 (1998)), low molecular weight heparins, GPIIb/IIIa antagonists (such as tirofiban), warfarin, thrombin inhibitors and carboxypeptidase U inhibitors (also known as inhibitors of active thrombin activatable fibrinolysis inhibitor [TAFIa]) (see Thrombosis Res. 101:329-354 (2001)). TAFIa inhibitors have been described in U.S. Serial Nos. 60/310,927 (filed August 8, 2001) and 60/349,925 (filed January 18, 2002).

(see, Nature Biotechnology, Vol. 17, pp.963-968 (October 1999); Kim et al., Nature,

362, 841-844 (1993); WO 00/44777; and WO 00/61186).

"Agents that interfere with cell cycle checkpoints" refer to compounds that inhibit protein kinases that transduce cell cycle checkpoint signals, thereby sensitizing the cancer cell to DNA damaging agents. Such agents include inhibitors of ATR, ATM, the Chk1 and Chk2 kinases and cdk and cdc kinase inhibitors and are specifically exemplified by 7-hydroxystaurosporin, flavopiridol, CYC202 (Cyclacel) and BMS-387032.

"Inhibitors of cell proliferation and survival signalling pathway" refer to compounds that inhibit signal transduction cascades downstream of cell surface receptors. Such agents include inhibitors of serine/threonine kinases (including but not limited to inhibitors of Akt such as described in WO 02/083064, WO 02/083139, WO 02/083140 and WO 02/083138), inhibitors of Raf kinase (for example BAY-43-9006), inhibitors of MEK (for example CI-1040 and PD-098059), inhibitors of mTOR (for example Wyeth CCI-779), and inhibitors of PI3K (for example LY294002).

The combinations with NSAID's are directed to the use of NSAID's which are potent COX-2 inhibiting agents. For purposes of this specification an NSAID is potent if it possess an IC₅₀ for the inhibition of COX-2 of $1\mu M$ or less as measured by cell or microsomal assays.

The invention also encompasses combinations with NSAID's which are selective COX-2 inhibitors. For purposes of this specification NSAID's which are 15 selective inhibitors of COX-2 are defined as those which possess a specificity for inhibiting COX-2 over COX-1 of at least 100 fold as measured by the ratio of IC50 for COX-2 over IC50 for COX-1 evaluated by cell or microsomal assays. Such compounds include, but are not limited to those disclosed in U.S. Patent 5,474,995, issued December 12, 1995, U.S. Patent 5,861,419, issued January 19, 1999, U.S. 20 Patent 6,001,843, issued December 14, 1999, U.S. Patent 6,020,343, issued February 1, 2000, U.S. Patent 5,409,944, issued April 25, 1995, U.S. Patent 5,436,265, issued July 25, 1995, U.S. Patent 5,536,752, issued July 16, 1996, U.S. Patent 5,550,142, issued August 27, 1996, U.S. Patent 5,604,260, issued February 18, 1997, U.S. 5,698,584, issued December 16, 1997, U.S. Patent 5,710,140, issued January 20,1998, 25 WO 94/15932, published July 21, 1994, U.S. Patent 5,344,991, issued June 6, 1994, U.S. Patent 5,134,142, issued July 28, 1992, U.S. Patent 5,380,738, issued January 10, 1995, U.S. Patent 5,393,790, issued February 20, 1995, U.S. Patent 5,466,823, issued November 14, 1995, U.S. Patent 5,633,272, issued May 27, 1997, and U.S. Patent 5,932,598, issued August 3, 1999, all of which are hereby incorporated by reference. 30

Inhibitors of COX-2 that are particularly useful in the instant method of treatment are:

3-phenyl-4-(4-(methylsulfonyl)phenyl)-2-(5H)-furanone; and

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5-chloro-3-(4-methylsulfonyl)phenyl-2-(2-methyl-5-pyridinyl)pyridine;

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or a pharmaceutically acceptable salt thereof.

General and specific synthetic procedures for the preparation of the COX-2 inhibitor compounds described above are found in U.S. Patent No. 5,474,995, issued December 12, 1995, U.S. Patent No. 5,861,419, issued January 19, 1999, and U.S. Patent No. 6,001,843, issued December 14, 1999, all of which are herein incorporated by reference.

Compounds that have been described as specific inhibitors of COX-2 and are therefore useful in the present invention include, but are not limited to, the following:

$$H_2N$$
 N CF_3 H_3C

$$H_3C$$
 N
 H_2N-S
 O
 O

or a pharmaceutically acceptable salt thereof.

Compounds which are described as specific inhibitors of COX-2 and are therefore useful in the present invention, and methods of synthesis thereof, can be found in the following patents, pending applications and publications, which are herein incorporated by reference: WO 94/15932, published July 21, 1994, U.S. Patent No. 5,344,991, issued June 6, 1994, U.S. Patent No. 5,134,142, issued July 28, 1992,
U.S. Patent No. 5,380,738, issued January 10, 1995, U.S. Patent No. 5,393,790, issued February 20, 1995, U.S. Patent No. 5,466,823, issued November 14, 1995, U.S. Patent No. 5,633,272, issued May 27, 1997, and U.S. Patent No. 5,932,598, issued August 3, 1999.

Compounds which are specific inhibitors of COX-2 and are therefore useful in the present invention, and methods of synthesis thereof, can be found in the following patents, pending applications and publications, which are herein incorporated by reference: U.S. Patent No. 5,474,995, issued December 12, 1995, U.S. Patent No. 5,861,419, issued January 19, 1999, U.S. Patent No. 6,001,843, issued December 14, 1999, U.S. Patent No. 6,020,343, issued February 1, 2000, U.S. Patent No. 5,409,944, issued April 25, 1995, U.S. Patent No. 5,436,265, issued July 25, 1995, U.S. Patent No. 5,536,752, issued July 16, 1996, U.S. Patent No. 5,550,142, issued August 27, 1996, U.S. Patent No. 5,604,260, issued February 18, 1997, U.S. Patent No. 5,698,584, issued December 16, 1997, and U.S. Patent No. 5,710,140, issued January 20,1998.

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Other examples of angiogenesis inhibitors include, but are not limited to, endostatin, ukrain, ranpirnase, IM862, 5-methoxy-4-[2-methyl-3-(3-methyl-2-butenyl)oxiranyl]-1-oxaspiro[2,5]oct-6-yl(chloroacetyl)carbamate, acetyldinanaline, 5-amino-1-[[3,5-dichloro-4-(4-chlorobenzoyl)phenyl]methyl]-1H-1,2,3-triazole-4-carboxamide,CM101, squalamine, combretastatin, RPI4610, NX31838, sulfated mannopentaose phosphate, 7,7-(carbonyl-bis[imino-N-methyl-4,2-pyrrole]-carbonylimino]-bis-(1,3-naphthalene disulfonate), and 3-[(2,4-dimethylpyrrol-5-yl)methylene]-2-indolinone (SU5416).

As used above, "integrin blockers" refers to compounds which selectively antagonize, inhibit or counteract binding of a physiological ligand to the $\alpha_V\beta_3$ integrin, to compounds which selectively antagonize, inhibit or counteract binding of a physiological ligand to the $\alpha_V\beta_5$ integrin, to compounds which antagonize, inhibit or counteract binding of a physiological ligand to both the $\alpha_V\beta_3$ integrin and the $\alpha_V\beta_5$ integrin, and to compounds which antagonize, inhibit or counteract the activity of the particular integrin(s) expressed on capillary endothelial cells. The term also refers to antagonists of the $\alpha_V\beta_6$, $\alpha_V\beta_8$, $\alpha_1\beta_1$, $\alpha_2\beta_1$, $\alpha_5\beta_1$, $\alpha_6\beta_1$ and $\alpha_6\beta_4$ integrins. The term also refers to antagonists of any combination of $\alpha_V\beta_3$, $\alpha_V\beta_5$, $\alpha_V\beta_6$, $\alpha_V\beta_8$, $\alpha_1\beta_1$, $\alpha_2\beta_1$, $\alpha_5\beta_1$, $\alpha_6\beta_1$ and $\alpha_6\beta_4$ integrins.

Some specific examples of tyrosine kinase inhibitors include N-(trifluoromethylphenyl)-5-methylisoxazol-4-carboxamide, 3-[(2,4-dimethylpyrrol-5-yl)methylidenyl)indolin-2-one, 17-(allylamino)-17-demethoxygeldanamycin, 4-(3-chloro-4-fluorophenylamino)-7-methoxy-6-[3-(4-morpholinyl)propoxyl]quinazoline, N-(3-ethynylphenyl)-6,7-bis(2-methoxyethoxy)-4-quinazolinamine, BIBX1382, 2,3,9,10,11,12-hexahydro-10-(hydroxymethyl)-10-hydroxy-9-methyl-9,12-epoxy-1H-

diindolo[1,2,3-fg:3',2',1'-kl]pyrrolo[3,4-i][1,6]benzodiazocin-1-one, SH268, genistein, STI571, CEP2563, 4-(3-chlorophenylamino)-5,6-dimethyl-7H-pyrrolo[2,3-d]pyrimidinemethane sulfonate, 4-(3-bromo-4-hydroxyphenyl)amino-6,7-dimethoxyquinazoline, 4-(4'-hydroxyphenyl)amino-6,7-dimethoxyquinazoline, SU6668, STI571A, N-4-chlorophenyl-4-(4-pyridylmethyl)-1-phthalazinamine, and EMD121974.

Combinations with compounds other than anti-cancer compounds are also encompassed in the instant methods. For example, combinations of the instantly claimed compounds with PPAR-y (i.e., PPAR-gamma) agonists and PPAR-S (i.e., PPAR-delta) agonists are useful in the treatment of certain malingnancies. PPAR-y and PPAR- δ are the nuclear peroxisome proliferator-activated receptors y and δ . The expression of PPAR-y on endothelial cells and its involvement in angiogenesis has been reported in the literature (see J. Cardiovasc. Pharmacol. 1998; 31:909-913; J. Biol. Chem. 1999;274:9116-9121; Invest. Ophthalmol Vis. Sci. 2000; 41:2309-2317). More recently, PPAR-y agonists have been shown to inhibit the angiogenic response to VEGF in vitro; both troglitazone and rosiglitazone maleate inhibit the development of retinal neovascularization in mice. (Arch. Ophthamol. 2001; 119:709-717). Examples of PPAR-y agonists and PPAR-y/\alpha agonists include, but are not limited to, thiazolidinediones (such as DRF2725, CS-011, troglitazone, rosiglitazone, and pioglitazone), fenofibrate, gemfibrozil, clofibrate, GW2570, SB219994, AR-H039242, JTT-501, MCC-555, GW2331, GW409544, NN2344, KRP297, NP0110. DRF4158, NN622, GI262570, PNU182716, DRF552926, 2-[(5,7-dipropyl-3trifluoromethyl-1,2-benzisoxazol-6-yl)oxyl-2-methylpropionic acid (disclosed in USSN 09/782,856), and 2(R)-7-(3-(2-chloro-4-(4-fluorophenoxy) phenoxy)-2-ethylchromane-2-carboxylic acid (disclosed in USSN 60/235,708 and 60/244,697).

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Another embodiment of the instant invention is the use of the presently disclosed compounds in combination with gene therapy for the treatment of cancer. For an overview of genetic strategies to treating cancer see Hall et al (Am J Hum Genet 61:785-789, 1997) and Kufe et al (Cancer Medicine, 5th Ed, pp 876-889, BC Decker, Hamilton 2000). Gene therapy can be used to deliver any tumor suppressing gene. Examples of such genes include, but are not limited to, p53, which can be delivered via recombinant virus-mediated gene transfer (see U.S. Patent No. 6,069,134, for example), a uPA/uPAR antagonist ("Adenovirus-Mediated Delivery of a uPA/uPAR Antagonist Suppresses Angiogenesis-Dependent Tumor Growth and

Dissemination in Mice," Gene Therapy, August 1998;5(8):1105-13), and interferon gamma (J. Immunol 2000;164:217-222).

The compounds designed or selected using the methods of the instant invention may also be administered in combination with an inhibitor of inherent multidrug resistance (MDR), in particular MDR associated with high levels of expression of transporter proteins. Such MDR inhibitors include inhibitors of p-glycoprotein (P-gp), such as LY335979, XR9576, OC144-093, R101922, VX853 and PSC833 (valspodar).

A compound designed or selected using the methods of the present 10 invention may be employed in conjunction with anti-emetic agents to treat nausea or emesis, including acute, delayed, late-phase, and anticipatory emesis, which may result from the use of a compound of the present invention, alone or with radiation therapy. For the prevention or treatment of emesis, a compound of the present invention may be used in conjunction with other anti-emetic agents, especially neurokinin-1 receptor antagonists, 5HT3 receptor antagonists, such as ondansetron, 15 granisetron, tropisetron, and zatisetron, GABAB receptor agonists, such as baclofen, a corticosteroid such as Decadron (dexamethasone), Kenalog, Aristocort, Nasalide, Preferid, Benecorten or others such as disclosed in U.S.Patent Nos. 2,789,118, 2,990,401, 3,048,581, 3,126,375, 3,929,768, 3,996,359, 3,928,326 and 3,749,712, an antidopaminergic, such as the phenothiazines (for example prochlorperazine, 20 fluphenazine, thioridazine and mesoridazine), metoclopramide or dronabinol. For the treatment or prevention of emesis that may result upon administration of the instant compounds, conjunctive therapy with an anti-emesis agent selected from a neurokinin-1 receptor antagonist, a 5HT3 receptor antagonist and a corticosteroid is 25 preferred.

Neurokinin-1 receptor antagonists of use in conjunction with the compounds of the present invention are fully described, for example, in U.S. Patent Nos. 5,162,339, 5,232,929, 5,242,930, 5,373,003, 5,387,595, 5,459,270, 5,494,926, 5,496,833, 5,637,699, 5,719,147; European Patent Publication Nos. EP 0 360 390, 0 394 989, 0 428 434, 0 429 366, 0 430 771, 0 436 334, 0 443 132, 0 482 539, 0 498 069, 0 499 313, 0 512 901, 0 512 902, 0 514 273, 0 514 274, 0 514 275, 0 514 276, 0 515 681, 0 517 589, 0 520 555, 0 522 808, 0 528 495, 0 532 456, 0 533 280, 0 536 817, 0 545 478, 0 558 156, 0 577 394, 0 585 913,0 590 152, 0 599 538, 0 610 793, 0 634 402, 0 686 629, 0 693 489, 0 694 535, 0 699 655,

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0 699 674, 0 707 006, 0 708 101, 0 709 375, 0 709 376, 0 714 891, 0 723 959, 0 733 632 and 0 776 893; PCT International Patent Publication Nos. WO 90/05525, 90/05729, 91/09844, 91/18899, 92/01688, 92/06079, 92/12151, 92/15585, 92/17449 92/20661, 92/20676, 92/21677, 92/22569, 93/00330, 93/00331, 93/01159, 93/01165. 5 93/01169, 93/01170, 93/06099, 93/09116, 93/10073, 93/14084, 93/14113, 93/18023 93/19064, 93/21155, 93/21181, 93/23380, 93/24465, 94/00440, 94/01402, 94/02461, 94/02595, 94/03429, 94/03445, 94/04494, 94/04496, 94/05625, 94/07843, 94/08997 94/10165, 94/10167, 94/10168, 94/10170, 94/11368, 94/13639, 94/13663, 94/14767, 94/15903, 94/19320, 94/19323, 94/20500, 94/26735, 94/26740, 94/29309, 95/02595. 10 95/04040, 95/04042, 95/06645, 95/07886, 95/07908, 95/08549, 95/11880, 95/14017, 95/15311, 95/16679, 95/17382, 95/18124, 95/18129, 95/19344, 95/20575, 95/21819. 95/22525, 95/23798, 95/26338, 95/28418, 95/30674, 95/30687, 95/33744, 96/05181, 96/05193, 96/05203, 96/06094, 96/07649, 96/10562, 96/16939, 96/18643, 96/20197 96/21661, 96/29304, 96/29317, 96/29326, 96/29328, 96/31214, 96/32385, 96/37489. 15 97/01553, 97/01554, 97/03066, 97/08144, 97/14671, 97/17362, 97/18206, 97/19084. 97/19942 and 97/21702; and in British Patent Publication Nos. 2 266 529, 2 268 931. 2 269 170, 2 269 590, 2 271 774, 2 292 144, 2 293 168, 2 293 169, and 2 302 689. The preparation of such compounds is fully described in the aforementioned patents and publications, which are incorporated herein by reference.

In an embodiment, the neurokinin-1 receptor antagonist for use in conjunction with the compounds of the present invention is selected from: 2-(R)-(1-(R)-(3.5-bis(trifluoromethyl)phenyl)ethoxy)-3-(S)-(4-fluorophenyl)-4-(3-(5-oxo-1H,4H-1,2,4-triazolo)methyl)morpholine, or a pharmaceutically acceptable salt thereof, which is described in U.S. Patent No. 5,719,147.

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A compound designed or selected using the methods of the instant invention may also be administered with an agent useful in the treatment of anemia. Such an anemia treatment agent is, for example, a continuous eythropoiesis receptor activator (such as epoetin alfa).

A compound designed or selected using the methods of the instant invention may also be administered with an agent useful in the treatment of neutropenia. Such a neutropenia treatment agent is, for example, a hematopoietic growth factor which regulates the production and function of neutrophils such as a human granulocyte colony stimulating factor, (G-CSF). Examples of a G-CSF include filgrastim.

A compound designed or selected using the methods of the instant invention may also be administered with an immunologic-enhancing drug, such as levamisole, isoprinosine and Zadaxin.

Thus, the scope of the instant invention encompasses the use of the compounds designed or selected using the methods disclosed herein in combination with a second compound selected from:

	was a second compo	and selected from.
	1)	an estrogen receptor modulator,
	2)	an androgen receptor modulator,
	3) .	retinoid receptor modulator,
10	4)	a cytotoxic/cytostatic agent,
	5)	an antiproliferative agent,
	6)	a prenyl-protein transferase inhibitor,
	7)	an HMG-CoA reductase inhibitor,
	8)	an HIV protease inhibitor,
15	9)	a reverse transcriptase inhibitor,
	10)	an angiogenesis inhibitor,
	11)	a PPAR-γ agonists,
	12)	a PPAR-δ agonists,
	13)	an inhibitor of inherent multidrug resistance,
20	14)	an anti-emetic agent,
	15)	an agent useful in the treatment of anemia,
	16)	an agent useful in the treatment of neutropenia,
	17)	an immunologic-enhancing drug,
	18)	an inhibitor of cell proliferation and survival signaling, and

The term "administration" and variants thereof (e.g., "administering" a compound) in reference to a compound of the invention means introducing the compound or a prodrug of the compound into the system of the animal in need of treatment. When a compound of the invention or prodrug thereof is provided in combination with one or more other active agents (e.g., a cytotoxic agent, etc.), "administration" and its variants are each understood to include concurrent and sequential introduction of the compound or prodrug thereof and other agents.

an agent that interfers with a cell cycle checkpoint.

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As used herein, the term "composition" is intended to encompass a product comprising the specified ingredients in the specified amounts, as well as any

product which results, directly or indirectly, from combination of the specified ingredients in the specified amounts.

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The term "therapeutically effective amount" as used herein means that amount of active compound or pharmaceutical agent that elicits the biological or medicinal response in a tissue, system, animal or human that is being sought by a researcher, veterinarian, medical doctor or other clinician.

The term "treating cancer" or "treatment of cancer" refers to administration to a mammal afflicted with a cancerous condition and refers to an effect that alleviates the cancerous condition by killing the cancerous cells, but also to an effect that results in the inhibition of growth and/or metastasis of the cancer.

In an embodiment, the angiogenesis inhibitor to be used as the second compound is selected from a tyrosine kinase inhibitor, an inhibitor of epidermal-derived growth factor, an inhibitor of fibroblast-derived growth factor, an inhibitor of platelet derived growth factor, an MMP (matrix metalloprotease) inhibitor, an integrin blocker, interferon- α , interleukin-12, pentosan polysulfate, a cyclooxygenase inhibitor, carboxyamidotriazole, combretastatin A-4, squalamine, 6-O-chloroacetyl-carbonyl)-fumagillol, thalidomide, angiostatin, troponin-1, or an antibody to VEGF. In an embodiment, the estrogen receptor modulator is tamoxifen or raloxifene.

Also included in the scope of the claims is a method of treating cancer that comprises administering a therapeutically effective amount of a compound designed or selected using the methods disclosed herein in combination with radiation therapy and/or in combination with a compound selected from:

- 1) an estrogen receptor modulator,
- 2) an androgen receptor modulator,
- a retinoid receptor modulator,
 - 4) a cytotoxic/cytostatic agent,
 - 5) an antiproliferative agent,
 - 6) a prenyl-protein transferase inhibitor,
 - 7) an HMG-CoA reductase inhibitor.
 - 8) an HIV protease inhibitor,
 - 9) a reverse transcriptase inhibitor,
 - 10) an angiogenesis inhibitor,
 - 11) PPAR-y agonists,
 - 12) PPAR-δ agonists,
- 35 an inhibitor of inherent multidrug resistance,

14) an anti-emetic agent,

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- 15) an agent useful in the treatment of anemia,
- 16) an agent useful in the treatment of neutropenia,
- 17) an immunologic-enhancing drug,
- 18) an inhibitor of cell proliferation and survival signaling, and
- 19) an agent that interfers with a cell cycle checkpoint.

And yet another embodiment of the invention is a method of treating cancer that comprises administering a therapeutically effective amount of a compound designed or selected using the methods disclosed herein in combination with paclitaxel or trastuzumab.

The invention further encompasses a method of treating or preventing cancer that comprises administering a therapeutically effective amount of a compound designed or selected using the methods disclosed herein in combination with a COX-2 inhibitor.

The instant invention also includes a pharmaceutical composition useful for treating or preventing cancer that comprises a therapeutically effective amount of a compound designed or selected using the methods disclosed herein and a compound selected from:

- 1) an estrogen receptor modulator,
- 20 an androgen receptor modulator,
 - 3) a retinoid receptor modulator,
 - 4) a cytotoxic/cytostatic agent,
 - 5) an antiproliferative agent,
 - 6) a prenyl-protein transferase inhibitor,
- 25 7) an HMG-CoA reductase inhibitor,
 - 8) an HIV protease inhibitor,
 - 9) a reverse transcriptase inhibitor,
 - 10) an angiogenesis inhibitor, and
 - 11) a PPAR-γ agonist,
- 30 12) a PPAR-δ agonists;
 - 13) an inhibitor of cell proliferation and survival signaling, and
 - 14) an agent that interfers with a cell cycle checkpoint.

In each of the aforementioned uses of atomic coordinates of KSP, the coordinates according to Tables 1-4 are preferred.

Additional objects of the present invention will be apparent from the description which follows.

As used herein, the following terms and phrases shall have the meanings set forth below:

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Unless otherwise noted, "KSP" includes both native and wild type Kinesin Spindle Protein as well as "KSP analogues", defined herein as proteins or peptides comprising a ligand binding site substantially as set forth in SEQ ID NO:1. Such KSP analogues include, but are not limited to, a ligand binding site characterized by a three-dimensional structure comprising the relative structural coordinates of amino acid residues set forth in Figure 10 as set forth in Tables 1-4, ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 3.005 Å, more preferably not more than about 2.0Å, and most preferably not more than about 0.5 Å.

Unless otherwise indicated, "protein" or "molecule" shall include a protein, protein domain, polypeptide or peptide.

"Structural coordinates" are the Cartesian coordinates corresponding to an atom's spatial relationship to other atoms in a molecule or molecular complex. Structural coordinates may be obtained using X-ray crystallography techniques or NMR techniques, or may be derived using molecular replacement analysis or homology modeling. Various software programs allow for the graphical representation of a set of structural coordinates to obtain a three-dimensional representation of a molecule or molecular complex. The structural coordinates of the present invention may be modified from the original sets provided in Tables 1-4 by mathematical manipulation, such as by inversion or integer additions or subtractions. As such, it is recognized that the structural coordinates of the present invention are relative, and are in no way specifically limited by the actual x, y, z coordinates of Tables 1-4.

An "agent", "ligand" or "binding partner" shall include a protein, polypeptide, peptide, nucleic acid, including DNA or RNA, molecule, compound or drug.

"Root mean square deviation" is the square root of the arithmetic mean of the squares of the deviations from the mean, and is a way of expressing deviation or variation from the structural coordinates

described herein. The present invention includes all embodiments comprising conservative substitutions of the noted amino acid residues resulting in same structural coordinates within the stated root mean square deviation.

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MATERIALS AND METHODS

Materials and methods provided are intended to assist in a further understanding of the invention and are not to limit the reasonable scope thereof.

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Motor Domain of Human KSP, Amino Acids 1-368

MASQPNSSAK KKEEKGKNIQ VVVRCRPFNL AERKASAHSI
VECDPVRKEV SVRTGGLADK SSRKTYTFDM VFGASTKQID
VYRSVVCPIL DEVIMGYNCT IFAYGQTGTG KTFTMEGERS

15 PNEEYTWEED PLAGIIPRTL HQIFEKLTDN GTEFSVKVSL
LEIYNEELFD LLNPSSDVSE RLQMFDDPRN KRGVIIKGLE
EITVHNKDEV YQILEKGAAK RTTAATLMNA YSSRSHSVFS
VTIHMKETTI DGEELVKIGK LNLVDLAGSE NIGRSGAVDK
RAREAGNINQ SLLTLGRVIT ALVERTPHVP YRESKLTRIL

20 QDSLGGRTRT SIIATISPAS LNLEETLSTL EYAHRAKNIL
NKPEVNOK

Binding Pocket of Human KSP

Lining the newly formed pocket and surrounding the ligand are amino acid residues:

115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P) (from helix- α 2 and its insertion loop; residue 116 is at the end of the first portion of helix- α 2 and residue 134 is at the beginning of the second portion of helix- α 2 thus the insertion loop starts at residue 116 and a decrease α 3.

30 and ends at residue 134);

160(L) (from beta strain- β 4); 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) (from helix- α 3); and 239(F) (from beta strain- β 6).

35 KSP Expression

E. coli cells harboring the KSP (368 residues) vector were grown at 37°C in LB medium containing 100 μg/ml ampicillin. KSP expression was induced at 25°C with 0.5mM isopropyl-D (–)-thiogalactopyranoside, and the cells were grown for four additional hours at 25°C prior to harvest.

Cells from 10 litre were suspended in 75 ml lysis buffer (50mM PIPES, 2mM MgCl₂, 1mM ATP, 1mM TCEP, 1mM EGTA, protease inhibitor tablets (one tablet per 50ml buffer)) and homogenized. Cells were disrupted by passing the homogenized suspension thrice through a Microfluidizer (Model 110-S). The cell lysate was centrifuged at 15,000 rpm for 30 minutes and the supernatant mixed with DE-52 resin (100 ml) pre-equilibrated in SP sepharose Buffer A (50mM PIPES, 2mM MgCl₂, 1mM ATP, 1mM TCEP, 1mM EGTA). Supernatant was removed after spinning at 1000 rpm for 10 minutes. Resin was washed twice with one resin volume (100ml) of 50mM PIPES, 2mM MgCl₂, 1mM ATP, 1mM TCEP, 1mM EGTA. The supernatants were pooled and loaded onto SP sepharose column (50ml, 2.6cm diameter column, Amersham Biosciences). Kinesin with ~95% purity was eluted at 0.15 to 0.2 M KCl using 0-30% KCl gradient. The fractions containing KSP (by SDS-PAGE analysis) were pooled and diluted with SP sepharose buffer A to a final KCl concentration of 50mM. The pool was mixed with 10ml of High performance Q-sepharose (Amersham Biosciencs) equilibrated in SP sepharose BufferA. The supernatent was collected by spinning at 1000rpm for 10 minutes. The resin was washed four times with two resin volume. The washes and supernatant were pooled and concentrated on Centriprep-10 to 15 to 17mg/ml and stored in small alicots at -70° C. The protein was characterized by N-terminal sequence analysis by Edman degradation on an Applied Biosystem model 470A gas phase sequencer. Protein concentration was determined with quantitative amino acid analysis by using a post column ninhydrin derivatization method on a Beckman 6300 analyzer. Molecular weight was determined on Deca-LCQ (Finnegan) mass spectrometer. Molar mass and size distribution was determined by multi-angle light scattering detector (Wyatt technology, DAWN EOS) connected to size exclusion column on Millenium HPLC.

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Crystallization

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The concentrated kinesin (ADP, Mg⁺⁺) protein at about 15mg/ml in 50mM PIPES buffer at pH 6.8 in the presence of 2mM MgCl₂, 1mM TECP, 1mM ATP, 84mM KCl, and 1mM EGTA was incubated with 1mM inhibitor Compound 5-2b ((+)-monastrol). Small single crystal seeds were obtained by hanging drop method with well solution containing 20% PEG3350, 0.15M K₂HPO₄ and 0.1M HEPES buffer at pH7.0 in about four days. Crystals suitable for X-ray data collection were obtained by macroseeding in hanging drops with well solution containing 14% PEG3350, 0.2M K₂HPO₄ and 0.1M HEPES at pH 6.8 in about two weeks. Hanging drops were formed by equal volume of protein and well solutions.

X-ray Data Collection and Procession

at 100K at synchrotron beamline 17-ID of the Advanced Photon Source at Argonne National Laboratory. Prior to data collection the crystal was soaked in the cryo-protectant solution for 20 minutes that contains 20% PEG3350, 0.15M K₂HPO₄, 20% PEG200, and 0.1M HEPES buffer at pH6.8. The crystal was then frozen in liquid nitrogen. The X-ray wavelength was set to 1Å. The data were collected at 0.2° oscillation per frame with 1000 frames total and 1 second exposure per frame at 250 mm detector to crystal distance. The data were processed and scaled by use of HKL2000 package. The crystal is in orthorhombic space group of P2₁2₁2₁ with cell dimensions of a= 69.5 Å b=79.5 Å and c=159.0 Å. The

Structure Determination and Refinement

The structure was determined by the use of the molecular replacement method in cooperation with extensive model rebuilding and dynamic refinement. The kinesin protein coordinates in the binary complex crystal structure of kinesin bound with ADP (Mg⁺⁺) was used as the search model. The molecular replacement solution was obtained with use of program AmoRe at 4.0Å to 15Å resolution range, which gave R-factor of 0.48 and correlation coefficient of 0.60. The initial protein model was

rebuilt and refined literally at 2.5Å resolution, those included dynamic refinement, energy minimization and temperature factor refinement. The Compound 5-2b density became apparent at the fourth rebuilding and refinement cycle. Finally, 441 water molecules were added in the model and the R-factor was 0.21 with R-free of 0.26 with good geometry (RMSD_{bonds} = 0.007 Å, RMSD_{angles} = 1.32°). The current protein model binds with one ADP, one Mg⁺⁺ ion and one Compound 5-2b. It starts at residue Asn18 to Lys362 with a gap from residue Asn271 to Asn287 (missing loop11 from Ile272 to Gly286) due to lack of electron density. There are two complexes in an asymmetric unit.

Tertiary Structure of KSP/ADP/Compound 5-2b

The 3-dimensional, tertiary structure of KSP, bound with Mg**-ADP and Compound 5-2b ((+)-monastrol), was determined at 2.5Å resolution with use of phases derived from a combination of molecular replacement, extensive manual rebuilding, and dynamic refinement. Two identical protein complexes were found in the asymmetric unit of the crystal and were related by a local, non-crystallographic 2-fold axis. For each, the electron density of the protein as well as those of the ligands (ADP, Mg**, and Compound 5-2b) was all well defined. Compound 5-2b was seen to be of the S handedness. Residues 2-17, 272-286, and 363-368 were disordered and showed no electron densities (The N-terminal Met1 residue was processed

25 Fluorescence of Trp127 of KSP(368)-ADP -/+ Inhibitors

upon expression). See Figures 1-8.

Materials

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- -2X kinesin buffer: 160 mM K-Hepes, 2 mM MgCl₂, 2 mM EGTA, 2 mM DTT (added fresh daily), and 100 mM KCl, pH 6.8.
- -Nucleotide: nucleotide is resuspended to 200 mM in 50 mM K-Hepes (pH6.8).
 - -Nucleotide is diluted 1:1 with 200 mM MgCl₂ to a stock concentration of 100 mM of 1:1 nucleotide:MgCl₂.
 - -Cuvette volume = $300 \mu l$

Methods

1) Add 281 μ l of 1X kinesin buffer, \pm nucleotide, and H₂O (Nucleotide = none, 1 mM AMPPNP, or 1 mM ADP (final concentration)).

- 5 2) Add 18.75 μl of 4 μM stock nucleotide-free KSP(367H).
 - 3) Add compound sequentially from DMSO stock (with all the volume of all additions \leq 0.6 μ l).
 - 4) Measure fluorescence after each addition (starting with buffer only).
- Example titration for Compound 8-1 with KSP(367H)ADP: 281 μl of 1X kinesin buffer + 1 mM ADP: add 250 nM KSP (18.75 μl of 4 uM nucleotide-free stock) add 1 nM Compound 8-1 (1 nM_f) (addition of 0.3 μl of 0.001 mM stock) add 2 nM Compound 8-1 (3 nM_f) (addition of 0.6 μl of 0.001 mM stock)
 add 4 nM Compound 8-1 (7 nM_f) (addition of 0.12 μl of 0.01 mM stock) add 3 nM Compound 8-1 (10 nM_f) (addition of 0.09 μl of 0.01 mM stock)
- add 3 nM Compound 8-1 (10 nM_f) (addition of 0.09 µl of 0.01 mM stock) add 20 nM Compound 8-1 (30 nM_f) (addition of 0.6 µl of 0.01 mM stock) add 40 nM Compound 8-1 (70 nM_f) (addition of 0.12 µl of 0.1 mM stock) add 30 nM Compound 8-1 (100 nM_f) (addition of 0.09 µl of 0.1 mM stock)
- add 200 nM Compound 8-1 (300 nM_f) (addition of 0.6 μl of 0.1 mM stock) add 400 nM Compound 8-1 (700 nM_f) (addition of 0.12 μl of 1 mM stock) add 300 nM Compound 8-1 (1000 nM_f) (addition of 0.09 μl of 1 mM stock) add 2000 nM Compound 8-1 (3000 nM_f) (addition of 0.6 μl of 1 mM stock).
 - 6) After each addition, measure steady-state fluorescence under the following conditions:
- 25 the following conditions:
 - $\lambda_{ex}=388$ nm, $\lambda_{em}=342\text{-}346$ nm, band width = 3 nm ex/3 nm em, wavelength increment = 0.5 nm, integration time = 2 s.
- Repeat the same titration series:
 in the absence of KSP (to determine compound-related background), and
 in the absence of KSP, but in the presence of 1 μM L-tryptophan (to determine compound-related effects on the amino acid itself).

Calculations

At the peak emission wavelength for W127 in KSP(367H) (=344 nm) measure the compound emission in kinesin buffer as a function of [compound]; measure fluorescence of L-tryptophan as a function of [compound]; measure fluorescence of KSP(367H) as a function of [compound]; correct KSP(367H) fluorescence for its decrease over time (due to losses of protein to the cuvette); subtract compound emission from L-tryptophan emission; subtract compound emission from KSP(367H) emission. Calculate the fraction of fluorescence of L-tryptophan vs [compound]: (L-trp fluorescence (344 nm) at given [compound]) / (L-trp fluorescence (344 nm) at given [compound]) / (KSP fluorescence (344 nm) at 0 cpd); then normalize: KSP (frcn fl) / L-trp(frcn fl) and plot vs [compound].

Results of this assay are illustrated in Figures 11-13.

Compounds that were utilized in the identification and testing of the novel KSP binding site that is disclosed herein may be prepared by the methods described below:

SCHEME 1

5 <u>Step 1</u>: 3-[3-(benzyloxy)phenyl]-1-(2-chlorophenyl)prop-2-en-1-one (1-4)

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To a solution of 2'-chloroacetophenone (1-1) (1.26mL, 9.70mmol) in 40 mL of THF at -78°C was slowly added 10.7 mL (10.7mmol) of a 1M LiHMDS solution in THF. After stirring for 1h at -78°C, a solution of 2.05g (9.70mmol) of 3-benzyloxy-benzaldehyde (1-2) in

8 mL of THF was added, and stirring was continued at that temperature for an additional hour. The mixture was then dumped into a separatory funnel containing 100 mL of saturated aqueous NH₄Cl and extracted twice with 100 mL of EtOAc. The organic phases were combined, washed with 100 mL of brine, and dried over Na₂SO₄. After filtering off the drying agent, the solvent was removed on a rotary evaporator, and the residue was dissolved in 50 mL of CH₂Cl₂. After cooling to -78°C, 4 mL of triethylamine and 2 mL of trifluoroacetic anhydride were added sequentially, and the mixture was allowed to warm to rt and stir for 12h. The reaction was then dumped into a separatory funnel with 100 mL of 1M HCl, the layers were separated, and the aqueous phase extracted again with CH₂Cl₂. The organic layers were combined, washed again with 1 M HCl, washed with water, and dried over Na₂SO₄. After concentration, the crude material was purified by chromatography on silica gel with a gradient of 0 to 40% EtOAc in hexanes over 45 min to provide 1-4 as a viscous yellow oil. Data for 1-4: ¹HNMR $(500 \text{ MHz}, \text{CDCl}_3) \delta 7.5 - 7.0 \text{ (m, 15H) } 5.1 \text{ (s, 2H) ppm.}$

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Step 2: 1-(2-chlorophenyl)-3-(hydroxyphenyl)prop-2-en-1-one (1-5)

To a solution of 740 mg (2.12mmol) of 1-4 in 15 mL of

20 CH₂Cl₂ at -78°C was added dropwise 2.75 mL (2.75mmol) of a 1M solution of BBr₃ in CH₂Cl₂. After stirring for 30 min at that temperature, 1 mL of MeOH was added, and the mixture was dumped into water, extracted twice with 50 mL of CH₂Cl₂, washed again with water, and dried over Na₂SO₄. After concentration, the residue was purified by column chromatography on silica gel with a gradient of 2 to 70% EtOAc in hexanes over 30 min to provide 1-5 as a beige solid. Data for 1-5: ¹HNMR (500 MHz, CDCl₃) 8 7.5 - 7.3 (m, 5H), 7.25 (m, 1H), 7.2 - 7.0 (m, 3H), 6.9 (m, 1H), 5.1 (bs, 1H) ppm.

30 Step 3: 3-[1-acetyl-3-(2-chlorophenyl)-4,5-dihydro-1H-pyrazol-5-yl]phenol (1-7)

To a solution of 120mg (0.46mmol) of chalcone 1-5 in 4 mL of acetic acid was added 50 μ L (0.93mmol) of hydrazine hydrate. The reaction was then placed in an oil bath at 110°C for 24h. After cooling to rt, the solvents were removed on a rotary evaporator, the residue was dissolved

in 50 mL of CH_2Cl_2 , washed twice with aqueous NaHCO₃, dried over Na₂SO₄, and concentrated. The residue was then purified by column chromatography on silica gel with a gradient of 5 to 75% EtOAc in hexanes over 30 min to provide 1-7 as a fluffy white solid. Data for 1-7: ¹HNMR (500 MHz, CDCl₃) δ 7.75 (m, 1H), 7.45 (m 1H), 7.4 – 7.3 (m, 2H), 7.2 (m, 1H), 6.8 (d, 1H), 6.7 (m, 2H), 5.5 (m, 1H), 3.9 (m, 1H), 3.3 (m, 1H), 2.4 (s, 3H) ppm. HRMS (ES) calc'd M + H for $C_{17}H_{15}ClN_2O_2$: 315.0895. Found: 315.0904.

WO 2004/004652

SCHEME 2

F NOBF₄

$$F$$
 NH_2
 $CH_3CN, 0 \, ^{\circ}C;$
 F
 N_2^+
 N_2^+

Step 1: 2,5-difluorobenzenediazonium tetrafluoroborate (2-1)

Nitrosonium tetrafluoroborate (905 mg, 7.75 mmol, 1.00
equiv) was added to a solution of 2,5-difluoroaniline (0.780 mL, 7.75 mmol, 1 equiv) in acetonitrile (50 mL) at 0°C. The resulting mixture was stirred for 1 h, then diluted with ethyl ether (150 mL). The precipitate was filtered and air-dried to give 2,5-difluorobenzenediazonium tetrafluoroborate (2-1) as a tan solid. ¹H NMR (300 MHz, CD₃OD) δ 8.54 (m, 1H), 8.24 (m, 1H), 7.95 (m, 1H).

10 <u>Step 2</u>: tert-butyl 3-(2,5-difluorophenyl)-2,3-dihydro-1H-pyrrole-1-carboxylate (2-2)

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Palladium(II) acetate (67 mg, 0.30 mmol, 0.020 equiv) was added to a vigourously stirred, deoxygenated mixture of tert-butyl 2,5dihydro-1H-pyrrole-1-carboxylate (2.59 mL, 15.0 mmol, 1 equiv) and 2,5difluorobenzenediazonium tetrafluoroborate (2-1, 3.42 g, 15.0 mmol, 1.00 equiv) in water and carbon tetrachloride (1:1, 150 mL) at 23°C, and the resulting mixture was stirred for 20 h. The reaction mixture was concentrated, and the residue partitioned between ethyl acetate (300 mL) and saturated aqueous sodium bicarbonate solution (75 mL). The organic layer was washed with brine, then dried over sodium sulfate and concentrated. The residue was dissolved in toluene (200 mL), and the resulting solution concentrated in vacuo to facilitate azeotropic removal of residual water. 2,6-Lutidine (3.50 mL, 30.0 mmol, 2.00 equiv) and trifluoroacetic anhydride (1.48 mL, 10.5 mmol, 0.700 equiv) were then sequentially added to a solution of the residue in toluene (100 mL) at -10°C. The resulting mixture was allowed to warm to 10 °C over 16 h, then heated at reflux for 1 h. The reaction mixture was allowed to cool to 23°C, then concentrated. The residue was partitioned between ethyl acetate (300 mL) and saturated aqueous sodium bicarbonate solution (150 mL). The organic layer was dried over sodium sulfate and concentrated. The residue was purified by flash column chromatography (hexanes initially, grading to 20% EtOAc in hexanes) to give tert-butyl 3-(2,5-difluorophenyl)-2,3-dihydro-1H-pyrrole-1carboxylate (2-2) as a red oil. ¹H NMR (500 MHz, CDCl₃) major rotamer: δ 7.03-6.84 (m, 3H), 6.70 (br s, 1H), 5.01 (br s, 1H), 4.42 (m, 1H), 4.13 (m, 1H), 3.60 (m, 1H), 1.50 (s, 9H).

Step 3: tert-butyl 4-(2,5-difluorophenyl)-2-phenyl-2,5-dihydro-1H-pyrrole-1-carboxylate (2-4)

Tris(dibenzylideneacetone)dipalladium(0) (59 mg, 064 mmol, 0.020 equiv) was added to a deoxygenated mixture of tert-butyl 3-(2,5-difluorophenyl)-2,3-dihydro-1H-pyrrole-1-carboxylate (2-2, 900 mg, 3.20 mmol, 1 equiv), benzenediazonium tetrafluoroborate (1-3, prepared by the method described above for 2-3, 614 mg, 3.20 mmol, 1.00 equiv), and sodium acetate trihydrate (1.32 g, 9.60 mmol, 3.00 equiv) in acetonitrile (70 mL) at 23°C. The reaction mixture was stirred for 16 h, then partitioned between saturated aqueous sodium bicarbonate solution and ethyl acetate (2 x 70 mL). The combined organic layers were dried over sodium sulfate and concentrated. The residue was purified by flash column chromatography (hexanes initially, grading to 40% hexanes in EtOAc) to provide tert-butyl 4-(2,5-difluorophenyl)-2-phenyl-2,5-dihydro-1H-pyrrole-1-carboxylate (2-4) as an orange oil. LRMS m/z (M+H-CH₃) 343.0 found, 343.1 required.

Step 4: 4-(2,5-difluorophenyl)-2-phenyl-2,5-dihydro-1H-pyrrole (2-5)

Trifluoroacetic acid (20 mL) was added to a solution of tert-butyl 4-(2,5-difluorophenyl)-2-phenyl-2,5-dihydro-1H-pyrrole-1-carboxylate (2-4, 700 mg, 1.96 mmol, 1 equiv) in dichloromethane (50 mL) at 23 °C, and the resulting mixture was stirred for 30 min, then concentrated to give 4-(2,5-difluorophenyl)-2-phenyl-2,5-dihydro-1H-pyrrole (2-5) as a TFA salt (brown oil). LRMS m/z (M+H) 258.1 found, 258.1 required.

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Step 5: 4-(2,5-difluorophenyl)-N,N-dimethyl-2-phenyl-2,5-dihydro-1H-pyrrole-1-carboxamide (2-6)

Triethylamine (1.37 mL, 9.79 mmol, 5.00 equiv) and dimethylcarbamoyl chloride (0.180 mL, 1.96 mmol, 1.00 equiv) were added to a solution of 4-(2,5-difluorophenyl)-2-phenyl-2,5-dihydro-1H-pyrrole (2-5, 1.96 mmol) in dichloromethane (50 mL) at 23°C, and the resulting mixture was stirred for 2 h, then concentrated. The residue was partitioned between saturated aqueous sodium bicarbonate solution (75 ml) and ethyl acetate (100 mL). The organic layer was dried over sodium sulfate and concentrated. The residue was purified by reverse-phase LC (H₂O/CH₃CN

gradient w/ 0.1 % TFA present) to provide 4-(2,5-difluorophenyl)-N,N-dimethyl-2-phenyl-2,5-dihydro-1H-pyrrole-1-carboxamide (2-6) as an off-white solid. 1 H NMR (500 MHz, CDCl₃) δ 7.35-7.29 (m, 4H), 7.25 (m, 1H), 7.05 (m, 1H), 7.00 (m, 1H), 6.96 (m, 1H), 6.40 (br s, 1H), 6.13 (m, 1H), 4.88 (ddd, 1H, J = 13.7, 5.6, 2.0 Hz), 4.52 (d, 1H, J = 13.7 Hz), 2.88 (s, 6H). LRMS m/z (M+H) 329.1 found, 329.1 required.

<u>Step 6</u>: Enantiomers of 4-(2,5-difluorophenyl)-N,N-dimethyl-2phenyl-2,5-dihydro-1H-pyrrole-1-carboxamide (2-7 and 2-8)

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Resolution of enantiomers of racemic 4-(2,5-difluorophenyl)-N,N-dimethyl-2-phenyl-2,5-dihydro-1H-pyrrole-1-carboxamide (2-6) by chiral normal-phase HPLC (Chiralcel OD column: 0.1 % diethylamine in 40% ethanol in hexanes) provided in order of elution 2-7 (-) and 2-8 (+).

SCHEME 3

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Step 1: (2S,4S)-tert-Butyl 4-hydroxy-2-phenylpyrrolidine-1-carboxylate (3-2)

To a flame dried flask equipped with stir bar was added tertbutyl (2S,4S)-4-{[tert-butyl(dimethyl)silyl]oxy}-2-phenylpyrrolidine-1carboxylate (3-1, prepared from (S)-(-)-4-chloro-3-hydroxybutyronotrile by the method of Maeda, et al Synlett 2001, 1808-1810, 7.8 g, 20.7 mmol) and anhydrous acetonitrile (20.0 mL). The resulting solution was treated with triethylamine trihydrofluoride (10.1 mL, 62.0 mmol) while stirring under N₂. The reaction stirred 12 h at 40 °C. The reaction was then diluted with EtOAc (100 mL) and poured into 5% aq. NaHCO3. Following cessation of gas evolution, the organic layer was washed three addition times with 5% aq. NaHCO₁. The organic layer was dried over magnesium sulfate, filtered and concentrated to provide crude product. Recrystallization was effected from EtOAc/hexanes to provide (2S,4S)-tert-butyl 4-hydroxy-2phenylpyrrolidine-1-carboxylate (3-2) as a white crystalline solid. ¹H NMR (300 MHz, CDCl₃) rotamers δ 7.38-7.18 (m, 5H), 4.90 (m, 1H), 4.42 (m, 1H), 3.88 (m, 1H), 3.56 (dd, J = 11.5, 4.0 Hz, 1H), 2.60 (m, 1H), 2.03 (m, 1H), 1.50 and 1.20 (br s, 9H); MS 208.0 found, 208.1 (M – C(CH₃)₃) required.

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Step 2: (2S)-tert-butyl 4-oxo-2-phenylpyrrolidine-1-carboxylate (3-3)

To a flame dried flask equipped with stir bar was added 150 mL anhydrous dichloromethane which was cooled to -78 °C. Oxalyl chloride (3.8 mL, 44 mmol) and DMSO (4.8 mL, 61 mmol) were added sequentially and the reaction stirred for 10 min. (2S,4S)-tert-butyl 4-hydroxy-2-phenylpyrrolidine-1-carboxylate (3-2, 2.28 g, 8.73 mmol) in 10 mL anhydrous dichloromethane was added dropwise and stirred 1 h at -78°C. Triethylamine (12 mL, 87mmol) was added and the reaction was warmed to 0°C over 1 h. Upon completion, the reaction was washed with 5% NaHCO₃, brine and dried over MgSO₄. The organic layer was concentrated to provide crude (2S)-tert-butyl 4-oxo-2-phenylpyrrolidine-1-carboxylate (3-3). Recrystallization was effected with EtOAc/hexanes. ¹H NMR (300 MHz, CDCl₃) δ 7.35 (m, 3H), 7.17 (m, 2H), 5.38 (m, 1H), 4.08 (d, J = 19.5 Hz, 1H), 3.90 (d, J = 19.3 Hz, 1H), 3.13 (dd, J = 18.8, 9.8 Hz,

1H), 2.58 (dd, J = 18.6, 2.4 Hz, 1H), 1.40 (br s, 9H); MS 206.0 found, 206.1 (M – C(CH₃)₃) required.

Step 3: (2S)-tert-butyl 2-phenyl-4-{[(trifluoromethyl)sulfonyl]oxy}-2,5-dihydro-1H-pyrrole-1-carboxylate (3-4)

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To a flame dried flask equipped with stir bar was added ketone (2S)-tert-butyl 4-oxo-2-phenylpyrrolidine-1-carboxylate (3-3, 0.16 g, 0.62 mmol) and anhydrous THF (2 mL). The resulting solution was cooled to -78 °C, and treated dropwise with lithium hexamethyldisilylamide (LHMDS, 0.68 mL, 1M in THF, 0.68 mmoL). The reaction stirred 1 h at -78 °C, and N-(5-chloropyridin-2-yl)-1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]-methanesulfonamide (0.27 g, 068 mmol) was added neat in one portion. The reaction was allowed to warm to 0 °C and stirred 4 hours total. The reaction was diluted with Et2O (10mL) and washed successively with H₂O (10mL) and brine (10 mL). The organic layer was dried over MgSO₄, filtered and concentrated. The crude residue was purified by flash column choromatography (0-20% EtOAc/hexanes gradient, 15 min) to provide (2S)-tert-butyl 2-phenyl-4-{[(trifluoromethyl)sulfonyl]oxy}-2,5dihydro-1H-pyrrole-1-carboxylate (3-4). H NMR (300 MHz, CDCl₃) major rotamer: δ 7.30 (m, 5H), 5.72 (m, 1H), 5.48 (m, 1H), 4.42 (m, 2H), 1.18 (s, 9H); MS 379.0 found 379.1 (M - CH₃) required.

Step 4: (2S)-4-(2,5-difluorophenyl)-2-phenyl-N,N-dimethyl-2,5dihydro-1H-pyrrole-1-carboxamide (3-5)

To a flame dried flask equipped with stir bar was added (2S)-tert-butyl 2-phenyl-4-{[(trifluoromethyl)sulfonyl]oxy}-2,5-dihydro-1H-pyrrole-1-carboxylate (3-4, 0.250 g, 0.636 mmol), 2,5-difluorophenyl boronic acid (0.251 g, 1.59 mmol), Na₂CO₃ (0.202 g, 1.91 mmol), and LiCl (0.081 g, 1.91 mmol). The solids were dissolved in 20 mL 4:1 DME/H₂O and degassed with nitrogen. Pd(PPh₃)₄ (0.037 g, 0.032 mmol) was added and the reaction was sealed under nitrogen and heated to 90 °C for 2 h. Upon completion, the reaction was partitioned between 5% aq. NaHCO₃ and EtOAc (3 x 50 mL), and the combined organic layers were dried over MgSO₄. Following filtration, the organic layer was concentrated and

purified via flash column chromatography (SiO₂, 0-20% EtOAc/hexanes gradient) to provide (2S)-tert-butyl 4-(2,5-difluorophenyl)-2-phenyl-2,5-dihydro-1H-pyrrole-1-carboxylate (3-5). Further transformations followed those described in Scheme 1 to provide the instant compound 2-6.

SCHEME 4

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Trans-1H-Imidazo[1',5':1,6]pyrido[3,4-b]indole-1,3(2H)-dione,5,6,11,11a-tetrahydro-2-methyl-5-(3-hydroxyphenyl) (4-2a)

To a mixture of DL-tryptophan (1.5 g, 7.44 mmol), 3-hydroxybenzaldehyde (0.90, 7.44 mmol) in EtOH (3 mL) was added aq. H₂SO₄ (14.9 mL of a 0.5 M solution). The reaction was heated to 50 C for 12 h. The reaction mixture was partly concentrated to remove EtOH and resuspended in H₂O (5 mL). The precipitate was collected by filtration and dried in vacuo. The portion of this solid residue (0.14 g, 0.47 mmol) was dissolved in acetone (3 mL) and treated with methyl isocyanate. The reaction mixture was heated at 150 C in a sealed vessel for 15 min in a microwave reactor. The reaction was cooled to r.t. and concentrated. The residue was absorbed onto silica gel then purified on an ISCO automated system affixed with a Biotage flash 40(s) cartridge eluting with 0-100% EtOAc in hexane at 20 mL/min over 30 min to afford a mixture of 4-2a/4-2b Trituration of this mixture with diethyl

ether provided pure $\underline{4-2a}$. Data for $\underline{4-2a}$: ¹HNMR (600 MHz, CD₃OD) δ 7.52 (d, J=8 hz, 1H), 7.27 (d, J=8 hz, 1H), 7.18 (m, 1H), 7.12 (m, 1H), 7.07 (m, 1H), 6.84 (m, 1H), 6.74 (m, 2H), 6.24 (s, 1H), 4.44 (m, 1H), 3.43 (m, 1H), 3.01 (s, 3H), 2.88 (m, 1H) ppm. HRMS Calcd (M+1) 348.1270; found 348.1343.

SCHEME 5

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(-)4-(3-Hydroxyphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydro-4H-pyrimidin-5-carboxylic acid ethyl ester (5-2a) and (+)-4-(3-Hydroxyphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydro-4H-pyrimidin-5-carboxylic acid ethyl ester (5-2b)

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Racemic monastrol (50 mg, Tocris) was resolved by chiral HPLC (Chiralpak AD column 5 x 50 cm; 20% EtOH/80% (hexanes + 0.1% diethylamine); flow = 60 mL/min) to yield (-)-enantiomer $\underline{1\text{-}2A}$ (R_T =57.0 min) and (+)-enantiomer $\underline{5\text{-}2B}$ (R_T = 71.2 min). Enantiomer $\underline{5\text{-}2B}$ was crystallized from hexanes to yield a yellow solid.

SCHEME 6

SCHEME 6 (continued)

SCHEME 6 (continued)

tert-Butyl 3-[(benzylamino)carbonyl]thien-2-ylcarbamate (6-2)

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A solution of tert-butyllithium in pentane (1.7 M, 42.5 mL, 72.3 mmol, 2.40 equiv) was added to a solution of tert-butyl thien-2-ylcarbamate (6-1, 6.00 g, 30.1 mmol, 1 equiv) in THF (300 mL) at -78 °C. The reaction mixture was stirred for 45 min, then solid CO₂ (approximately 20 g) was added and the resulting mixture was warmed to 0 °C and stirred for 30 minutes. The reaction mixture was partitioned between aqueous 1 N hydrochloric acid solution and ethyl acetate (2 x 150 mL). The combined organic layers were dried over sodium sulfate and concentrated. The residue

was purified by flash column chromatography (hexanes initially, grading to 100% ethyl acetate), and the polar fractions were concentrated. A solution of the residue, benzylamine (6.61 g, 61.7 mmol, 2.05 equiv), 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (5.91 g, 30.8 mmol, 1.02 equiv), 1-hydroxy-7-azabenzotriazole (4.19 g, 30.8 mmol, 1.02 equiv), and triethylamine (8.59 mL, 61.7 mmol, 2.05 equiv) in DMF (100 mL) was stirred at 55°C for 24 h. The reaction mixture was concentrated, and the residue was partitioned between saturated aqueous sodium bicarbonate solution and ethyl acetate (3 x 100 mL). The combined organic layers were dried over sodium sulfate and concentrated. The residue was purified by flash column (hexanes initially, grading to 100% ethyl acetate) to give tert-butyl 3-[(benzylamino)carbonyl]thien-2-ylcarbamate (6-2) as a colorless oil. 1 H NMR (300 MHz, CDCl₃) δ 7.37 (m, 5H), 6.87 (d, 1H, J = 5.8 Hz), 6.69 (d, 1H, J = 5.8 Hz), 6.13 (s, 1H), 4.61 (d, 2H, J = 5.5 Hz), 1.52 (s, 9H).

N-benzyl-2-(butyrylamino)thiophene-3-carboxamide (6-3)

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A solution of tert-butyl 3-[(benzylamino)carbonyl]thien-2-ylcarbamate (6-2, 500 mg, 1.50 mmol, 1 equiv) was saturated with HCl gas at 0 °C, and the resulting solution was stirred at 0 °C for 1 h, then allowed to warm to 23 °C and stirred for 1 h. The reaction mixture was concentrated and the residue was dissolved in pyridine (10 mL). The resulting solution was cooled to 0 °C, and butyryl chloride (420 μ L, 4.04 mmol, 2.69 equiv) was added in three equal portions over 1 h. The reaction mixture was partitioned between aqueous sodium bicarbonate solution and ethyl acetate (50 mL). The organic layer was dried over sodium sulfate and concentrated. The residue was purified by flash column (hexanes initially, grading to 100% ethyl acetate) to give N-benzyl-2-(butyrylamino)thiophene-3-carboxamide (6-3) as an off-white solid. ¹H NMR (300 MHz, CDCl₃) δ 7.36 (m, 5H), 6.92 (d, 1H, J = 6.1 Hz), 6.76 (d, 1H, J = 5.8 Hz), 6.23 (s, 1H), 4.62 (d, 2H, J = 5.8 Hz), 2.47 (t, 2H, J = 7.3 Hz), 1.80 (sextet, 2H, J = 7.3 Hz), 1.01 (t, 3H, J = 7.3 Hz).

3-benzyl-2-propylthieno[2,3-d]pyrimidin-4(3H)-one (6-4)

A mixture of N-benzyl-2-(butyrylamino)thiophene-3-carboxamide (6-3, 230 mg, 0.76 mmol, 1 equiv) and sodium hydroxide (3 mg, 0.08 mmol, 0.1 equiv) in ethylene glycol (5 mL) was heated at 130 °C for 5 h. The reaction mixture was allowed to cool, then partitioned between a half-saturated aqueous sodium chloride solution and ethyl acetate (2 x 75 mL). The combined organic layers were dried over sodium sulfate and concentrated. The residue was purified by flash column (hexanes initially, grading to 100% ethyl acetate) to provide 3-benzyl-2-propylthieno[2,3-d]pyrimidin-4(3H)-one (6-4) as a colorless oil which solidified upon standing. ¹H NMR (300 MHz, CDCl₃) δ 7.48 (d, 1H, *J* = 5.8 Hz), 7.31 (m, 3H), 7.19 (d, 1H, *J* = 5.8 Hz), 7.17 (d, 2H, *J* = 7.9 Hz), 5.42 (s, 2H), 2.72 (t, 2H, *J* = 7.6 Hz), 1.78 (sextet, 2H, *J* = 7.6 Hz), 0.97 (t, 3H, *J* = 7.3 Hz).

3-benzyl-5,6-dibromo-2-(1-bromopropyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-5) and 3-benzyl-6-bromo-2-(1-bromopropyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-6)

A solution of 3-benzyl-2-propylthieno[2,3-d]pyrimidin-4(3H)-one (6-4, 100 mg, 0.35 mmol, 1 equiv), potassium acetate (207 mg, 20 2.1 mmol, 6 equiv) and bromine (338 mg, 2.1 mmol, 6 equiv) in acetic acid (2 mL) was heated at 100°C for 3 hr. The reaction was concentrated, and the residue was purified by flash chromatography. Elution with 30 % hexanes/EtOAc gave 3-benzyl-5,6-dibromo-2-(1-bromopropyl)thieno[2,3d]pyrimidin-4(3H)-one (6-5) as a colorless solid. ¹H NMR (500 MHz, 25 CDCl₃) δ 7.30 (m, 1H), 7.14 (d, J = 7.3 Hz, 2H), 6.19 (d, J = 16.3 Hz, 1H), 4.87 (d, J = 16.3 Hz, 1H), 4.62 (t, J = 7.3 Hz, 1H), 2.35 (m, 1H), 2.18 (m, J= 1H), 0.72 (t, J = 7.3 Hz, 3H). Further elution with the same eluant gave 3benzyl-6-bromo-2-(1-bromopropyl)thieno[2,3-d]pyrimidin-4(3H)-one (2-6) as a colorless gum. ¹H NMR (500 MHz, CDCl₃) δ 7.53 (s, 1H), 7.34 (m, 30 2H), 7.29 (m, 1H), 7.12 (d, J = 7.3 Hz, 2H), 6.21 (d, J = 16.3 Hz, 1 H), 4.88 (d, J = 16.3 Hz, 1H), 4.62 (t, J = 7.2 Hz, 1H), 2.37 (m, 1H), 2.18 (m, 1H),0.72 (t, J = 7.3 Hz, 3H).

3-benzyl-5,6-dibromo-2-(1-{[2-(dimethylamino)ethyl]amino}propyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-7)

A solution of 3-benzyl-5,6-dibromo-2-(1-

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bromopropyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-5, 35 mg, 0.066 mmol, 1 equiv) and N,N-dimethylethylenediamine (17 mg, 0.198 mmol, 3 equiv) in ethanol (5mL) was heated at reflux for 18 h. The reaction was concentrated, and the residue was partitioned between EtOAc and brine. The organic layer was dried (MgSO₄) and concentrated to provide 3-benzyl-5,6-dibromo-2-(1-{[2-(dimethylamino)ethyl]amino}propyl)thieno-[2,3-d]pyrimidin-4(3H)-one (6-7) as a yellow gum. MS(M+1) = 526.8.

3-benzyl-6-bromo-2-(1-{[2-(dimethylamino)ethyl]amino}propyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-8)

A solution of 3-benzyl-6-bromo-2-(1-bromopropyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-6, 35 mg, 0.079 mmol, 1 equiv) and N,N-dimethylethylenediamine (21 mg, 0.237 mmol, 3 equiv) in ethanol (5mL) was heated at reflux for 18 h. The reaction was concentrated, and the residue was partitioned between EtOAc and brine. The organic layer was dried (MgSO₄) and concentrated to provide 3-benzyl-6-bromo-2-(1-{[2-(dimethylamino)ethyl]amino}-propyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-8) as a yellow gum. MS(M+1) = 449.9.

N-[1-(3-benzyl-5,6-dibromo-4-oxo-3,4-dihydrothieno[2,3-d]pyrimidin-2-yl)propyl]-4-bromo-N-[2-(dimethylamino)ethyl]benzamide (6-9)

A solution of 4-bromobenzoyl chloride (19 mg, 0.085 mmol,

1 equiv) in dichloromethane (1 mL) was added to a solution of 3-benzyl-5,6-dibromo-2-(1-{[2-(dimethylamino)ethyl]amino}propyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-8, 45 mg, 0.085 mmol, 1 equiv) and N,N-diisopropylethylamine (11 mg, 0.085 mmol, 1 equiv) in dichloromethane (5 mL), and the resulting reaction mixture was stirred under ambient conditions for 1 h. The reaction mixture was washed with saturated aqueous NaHCO₃ solution, then brine, and dried (MgSO₄) and concentrated. The residue was purified by reverse-phase LC (H₂O/CH₃CN gradient w/ 0.1 % TFA present) to provide N-[1-(3-benzyl-5,6-dibromo-4-oxo-3,4-dihydrothieno[2,3-

d]pyrimidin-2-yl)propyl]-4-bromo-N- $\{2-(dimethylamino)ethyl\}$ benzamide (6-9) as a colorless foam. MS(M+1) = 708.9

N-[1-(3-benzyl-6-bromo-4-oxo-3,4-dihydrothieno[2,3-d]pyrimidin-2-yl)propyl]-4-bromo-N-[2-(dimethylamino)ethyl]benzamide (6-10)

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A solution of 4-bromobenzoyl chloride (19 mg, 0.085 mmol, 1 equiv) in dichloromethane (1 mL) was added to a solution of 3-benzyl-6-bromo-2-(1-{[2-(dimethylamino)ethyl]amino}propyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-9, 38 mg, 0.085 mmol, 1 equiv) and N,N-

diisopropylethylamine (11 mg, 0.085 mmol, 1 equiv) in dichloromethane (5 mL), and the resulting reaction mixture was stirred under ambient conditions for 1 h. The reaction mixture was washed with saturated aqueous NaHCO₃ solution, and brine, then dried (MgSO₄) and concentrated. The residue was purified by reverse-phase LC (H₂O/CH₃CN gradient w/ 0.1 % TFA present)

to provide N-[1-(3-benzyl-6-bromo-4-oxo-3,4-dihydrothieno[2,3-d]pyrimidin-2-yl)propyl]-4-bromo-N-[2-(dimethylamino)ethyl]benzamide (6-10) as a colorless foam. ¹H NMR (500 MHz, CDCl₃) δ 7.55 (m, 3H), 7.31 (m, 5H), 7.14 (m, 2H), 6.04 (d, J = 15.4 Hz, 1H), 5.92 (m, 1H), 5.12 (d, J = 15.4 Hz, 1H), 3.37 (m, 2H), 2.05 (m, 4 H), 1.83 (m, 6H), 0.65 (m, 3H).

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SCHEME 7

5 3-benzyl-2-(1-{[2-(dimethylamino)ethyl]amino}propyl)thieno[2,3-d]pyrimidin-4(3H)-one (7-1)

A mixture of 3-benzyl-6-bromo-2-(1-{[2-(dimethylamino)ethyl]-amino}propyl)-thieno[2,3-d]pyrimidin-4(3H)-one (6-8,17 mg, 0.38 mmol, 1 equiv) and 10 % Pd/C in ethyl acetate (5 mL) was hydrogenated at 1 atm. for 3 h. The mixture was filtered and the filtrate concentrated to provide 3-benzyl-2-(1-{[2-

(dimethylamino)ethyl]amino]propyl)thieno[2,3-d]pyrimidin-4(3H)-one (7-1) as a pale yellow gum. MS(M+1) = 371.1.

N-[1-(3-benzyl-4-oxo-3,4-dihydrothieno[2,3-d]pyrimidin-2-yl)propyl]-4-bromo-N-[2-(dimethylamino)ethyl]benzamide (7-2)

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A solution of 4-bromobenzoyl chloride (8 mg, 0.035 mmol, 1 equiv) in dichloromethane (1 mL) was added to a solution of 3-benzyl-2-(1-{[2-(dimethylamino)ethyl]amino}propyl)thieno[2,3-d]pyrimidin-4(3H)-one (7-1, 13 mg, 0.035 mmol, 1 equiv) and N,N-diisopropylethylamine (5 mg, 0.035 mmol, 1 equiv) in dichloromethane (1 mL), and the resulting mixture was stirred under ambient conditions for 1 h. The reaction mixture was washed with saturated aqueous NaHCO₃ solution, and brine, then dried (MgSO₄) and concentrated. The residue was purified by flash chromatography. Elution with CH₂Cl₂ to 5 % NH₃-EtOH/CH₂Cl₂ gave N-{1-(3-benzyl-4-oxo-3,4-dihydrothieno[2,3-d]pyrimidin-2-yl)propyl]-4-bromo-N-[2-(dimethylamino)ethyl]benzamide (7-2) as an off-white foam. ¹H NMR (500 MHz, CDCl₃) δ 7.31 (m, 5H), 7.14 (m, 2H), 6.09 (d, *J* = 15.6 Hz, 1H), 5.94 (m, 1H), 5.10 (d, *J* = 15.6 Hz, 1H), 3.40 (m, 2H), 2.11 (m, 1H), 2.03 (m, 2H), 1.87 (m, 1H), 1.79 (s, 6H), 0.66 (t, *J* = 6.6 Hz, 3H).

SCHEME 8

3-benzyl-2-(1-{(4-bromobenzyl)[2-(dimethylamino)ethyl]amino}propyl)thieno[2,3-d]pyrimidin-4(3H)-one(8-1)

A solution of 3-benzyl-2-(1-{[2-

- (dimethylamino)ethyl]amino}-propyl)thieno[2,3-d]pyrimidin-4(3H)-one(7-5 1, 175 mg, 0.47 mmol, 1 equiv) and 4-bromobenzaldehyde (174 mg, 0.94 mmol, 2 equiv) in methanol (20 mL) was treated with a solution of sodium cyanoborohydride in tetrahydrofuran (1 M, 0.94 mL, 0.94 mmol, 2 equiv). Acetic acid was added to obtain a pH of 6-7 and the reaction was warmed at 60 °C for 18 h. An additional 2 equivalents of 4-bromobenzaldehyde and 10 sodium cyanoborohydride were added after 18, 42 and 66 hours while maintaining the pH at 6-7 with acetic acid. After warming 90 h at 60°C, the reaction was concentrated and the residue was partitioned between EtOAc and aqueous saturated NaHCO3 solution. The organic layer was washed with brine, dried (MgSO₄) and concentrated. The residue was purified by flash 15 chromatography. Elution with EtOAc to 5 % NH3-EtOH/EtOAC gave 3benzyl-2-(1-{(4-bromobenzyl)[2-(dimethylamino)ethyl]amino)propyl)thieno[2,3-d]pyrimidin-4(3H)-one(8-1)as a pale yellow gum. ¹H NMR (500 MHz, CDCl₃) δ 7.45 (d, J = 6 Hz, 1H),
- 20 7.33 (d, J = 8 Hz, 2H), 7.21 (m, 4H), 7.05 (d, J = 8 Hz, 2H), 6.84 (d, J = 7 Hz, 2H), 5.85 (d, J = 16 Hz, 1H), 5.32 (d, J = 16 Hz, 1H), 3.87 (d, J = 14 Hz, 1H), 3.73 (dd, J = 11, 3 Hz, 1H), 3.50 (d, J = 14 Hz, 1H), 2.92 (m, 1H), 2.61 (m, 1H), 2.28 (m, 2H), 2.15 (m, 1H), 2.07 (s, 6H), 1.74 (m, 1H), 0.64 (t, J = 7 Hz, 3H).

TABLE I

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                                   22
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25.588
                                                      -5.423 104.627
                                                                         1.00 15.50
                      CG1 VAL
                                   22
                                                      -5.628 105.201
       ATOM
                 36
                                                                         1.00 16.80
50
        ATOM
                      CG2 VAL
                                   22
                                             23.817
                                                      -3.968 104.623
                                                                         1.00 15.97
       MOTA
                 38
                      C
                           VAL
                                   22
                                             22.838
                                                      -5.518 102.532
                                                                         1.00 13.29
       ATOM
                 39
                      0
                           VAI.
                                   22
                                             22.811
                                                      -4.469 101.884
                                                                         1.00 13.40
                 40
                           VAL
                      N
       MOTA
                                   23
                                             21.773
                                                      -6.292 102.694
-5.953 102.125
                                                                         1.00 12.04
                                   23
                                             20.478
       MOTA
                 41
                      CA
                           VAL
                                                                         1.00 11.16
55
       MOTA
                  42
                      СВ
                           VAL
                                             19.890
                                                      -7.155 101.350
                                                                         1.00 10.39
                      CG1 VAL
       MOTA
                 43
                                   23
                                             18.423
                                                      -6.883 100.979
                                                                         1.00
                                                                                6.97
       ATOM
                 44
                                   23
23
                                             20.733
                                                      -7.429 100.112
                                                                         1.00
                                                                                5.75
                 45
                           VAL
       MOTA
                      C
                                             19.496
19.433
                                                                         1.00 12.26
                                                      -5.551 103.220
                                   23
                                                      -6.180 104.276
       MOTA
                           VAL
                                                                         1.00 12.72
60
                                             18.734
17.741
       ATOM
                 47
                           ARG
                                                      -4.497 102.965
                                                                         1.00
       ATOM
                 48
                      CA
                           ARG
                                   24
                                                      -4.033 103.925
                                                                         1.00 11.98
                           ARG
       ATOM
                 49
                      CB
                                   24
                                             18.150
                                                      -2.711 104.572
                                                                         1.00
                                                                               9.94
       ATOM
                 50
                      CG
                           ARG
                                   24
                                             17.092
17.412
                                                      -2.197 105.533
                                                                         1.00
                                                                                9.40
       MOTA
                      CD
                           ARG
                                   24
                                                      -0.826 106.110
                                                                         1.00 11.24
65
       ATOM
                 52
                      NE
                           ARG
                                   24
                                                                         1.00
                                             16.638
                                                      -0.585 107.326
                                                                                8.87
       ATOM
                 53
                      CZ
                           ARG
                                             16.668
                                                       0.540 108.033
                                                                         1.00 11.40
                      NH1
                          ARG
       ATOM
                 54
                                   24
                                             17.432
                                                       1.563 107.649
                                                                         1.00 11.52
                 55
                      NH2 ARG
       MOTA
                                   24
                                                                         1.00 12.63
                                             15.956
                                                       0.629 109.151
                                                                                            Α
       MOTA
                 56
                      С
                           ARG
                                   24
                                             16.404
                                                      -3.831 103.230
                                                                         1.00 13.62
                                                                                            Α
70
       MOTA
                 57
                      0
                           ARG
                                   24
                                             16.248
                                                      -2.918 102.415
       MOTA
                 58
                           CYS
                                                      -4.690 103.553
                                                                         1.00 12.77
```

	MOTA	59	ÇA	CYS	25	14.117	-4.599	102.983	1.00 13.88	A
	MOTA	60	CB	CYS	25	13.461	-5 980	102.951	1.00 15.60	A
		61	SG	CYS	25				1.00 21.58	A
	MOTA					11.855		102.134		
_	MOTA	62	С	CYS	25	13.292	-3.675	103.865	1.00 13.78	A
5	MOTA	63	0	CYS	25	13.293	-3.820	105.084	1.00 15.62	A
	MOTA	64	N	ARG	26	12.605	-2.713	103.261	1.00 12.12	A
	MOTA	65	CA	ARG	26	11.774		104.045	1.00 12.61	λ
	MOTA	66	CB	arg	26	11.601	-0.465	103.343	1.00 10.76	A
	ATOM	67	CG	ARG	26	10.679	-0.499	102.128	1.00 7.66	A
10	MOTA	68	CD	ARG	26	10.181		101.775	1.00 7.16	A
10										
	MOTA	69	NE	ARG	26	9.592		100.442	1.00 7.55	A
	MOTA	70	CZ	ARG	26	8.413	0.411	100.125	1.00 8.80	A
	MOTA	71	NH1	ARG	26	7.677	-0.194	101.052	1.00 8.81	A
	MOTA	72	NH2		26	7.980	0.472	98.876	1.00 7.02	A
15										
13	MOTA	73	c	ARG	26	10.407		104.215	1.00 15.65	A
	MOTA	74	0	ARG	26	10.058	-3.420	103.500	1.00 17.10	A
	MOTA	75	N	PRO	27	9.615	-1.982	105.170	1.00 17.31	A
	MOTA	76	CD	PRO	27	9.957		106.262	1.00 18.01	A
20	MOTA	77	CA	PRO	27	8.287		105.382	1.00 20.54	A
20	MOTA	78	CB	PRO	27	8.037	-2.277	106.858	1.00 19.92	A
	MOTA	79	CG	PRO	27	8.639	-0.932	107.017	1.00 17.88	A
	MOTA	80	С	PRO	27	7.237		104.492	1.00 23.41	A
	MOTA	81	ŏ	PRO	27	7.482		103.916	1.00 23.28	A
~~	MOTA	82	N	PHE	28	6.080	-2.542	104.371	1.00 26.52	A
25	MOTA	83	CA	PHE	28	4.976	-2.003	103.584	1.00 29.18	A
	MOTA	84	CB	PHE	28	3.805	-2.982	103.588	1.00 27.65	A
	MOTA	85		PHE	28	3.948		102.610	1.00 28.35	A
									1.00 28.03	
	MOTA	86	CD1		28	3.947		103.045		A
~~	MOTA	87	CD2	PHE	28	4.038	-3.850	101.243	1.00 27.68	A
30	MOTA	88	CEl	PHE	28	4.026	-6.477	102.139	1.00 27.56	A
	MOTA	89	CE2	PHE	28	4.119	-4.893	100.324	1.00 29.26	A
	MOTA	90	cz	PHE	28	4.112		100.773	1.00 27.81	A
	MOTA	91	С	PHE	28	4.513		104.191	1.00 32.56	λ
0.5	ATOM.	92	0	PHE	28	4.426		105.411	1.00 33.43	A
35	MOTA	93	N	ASN	29	4.217	0.299	103.345	1.00 37.21	A
	MOTA	94	CA	ASN	29	3.744	1.595	103.829	1.00 42.32	A
	MOTA	95	СВ	ASN	29	4.073		102.809	1.00 42.04	A
	MOTA	96			29			101.410	1.00 41.31	A
			CG	ASN		3.604				
ďΔ	MOTA	97	ODI		29	2.409		101.168	1.00 41.82	À
40	MOTA	98	ND2	ASN	29	4.546	2.228	100.482	1.00 40.11	A
	MOTA	99	С	ASN	29	2.232	1.526	104.054	1.00 46.51	A
	MOTA	100	0	ASN	29	1.606		103.768	1.00 46.59	A
	MOTA	101	N	LEU	30	1.650		104.562	1.00 51.19	A
15	MOTA	102	CA	LEU	30	0.212		104.826	1.00 54.81	A
45	MOTA	103	CB	LEU	30	-0.178	4.040	105.362	1.00 56.40	A
	MOTA	104	CC	LEU	30	-1.659	4.234	105.705	1.00 58.19	A
	MOTA	105	CD1	LEU	30	-2.058	3.273	106.820	1.00 57.83	A
	MOTA	106	CD2		30	-1.899		106.130	1.00 59.11	A
50	MOTA	107	C	LEU	30	-0.637		103.592	1.00 56.70	A
50	MOTA	108	0	LEU	30	-1.552		103.658	1.00 56.66	A
	MOTA	109	N	ALA	31	-0.329	2.992	102.471	1.00 59.03	A
	MOTA	110	CA	ALA	31	-1.062	2.787	101.222	1.00 61.19	A
	ATOM	111		ALA	31	-0.414		100.100	1.00 61.28	A
55	MOTA	112		ALA	31	-1.125		100.833	1.00 62.78	Α
55	MOTA	113	0	ALA	31	-2.123	0.850	100.282	1.00 62.16	A
	MOTA	114	N	GLU	32	-0.048	0.593	101.117	1.00 65.22	A
	MOTA	115	CA	GLU	32	0.031	-0.827	100.801	1.00 67.27	A
	ATOM	116		GLU	32	1.501		100.702	1.00 66.96	A
۷۸	MOTA	117		GLU	32	2.199	-0.712	99.453	1.00 67.12	A
60	MOTA	118	CD	GLU	32	3.713	-0.641	99.590	1.00 67.26	A
	MOTA	119	0E1	GLU	32	4.392	-0.422	98.563	1.00 66.83	λ
	ATOM	120	OE2	GLU	32	4.223	-0.792	100.723	1.00 65.99	A
	ATOM	121		GLU	32	-0.706		101.844	1.00 68.26	A
65	MOTA	122		GLU	32	-1.260		101.526	1.00 68.16	A
65	MOTA	123		ARG	33	-0.722		103.087	1.00 69.65	A
	MOTA	124	CA	ARG	33	-1.403	-1.897	104.169	1.00 71.22	A
	ATOM	125		ARG	33	-1.196		105.498	1.00 72.33	A
	MOTA	126		ARG	33	0.239		106.009	1.00 73.65	A
70	ATOM	127		ARG	33	0.695		106.479	1.00 74.57	A
70	MOTA	128		ARG	33	2.043		107.041	1.00 76.44	A
	MOTA	129	CZ	ARG	33	2.692	-3.517	107.521	1.00 76.91	A
	ATOM	130	NH1		33	2.119		107.513	1.00 76.68	A
	ATOM	131	NH2		33	3.918		108.007	1.00 77.35	Ä
		-71	12		,,	2.310	- 3 . 3 , 6	100.007	1.00 17.33	^

										_
•	MOTA	132	C	ARG	33	-2.901		103.885	1.00 71.74	A
	MOTA	133	0	ARG	33	-3.464		103.900	1.00 71.46	A
	ATOM	134	N	LYS	34	-3.536		103.632	1.00 71.80	A
5	MOTA	135	CA	LYS	34 34	-4.967 -5.426		103.349	1.00 71.87	A A
5	MOTA MOTA	136 137	CB CG	LYS LYS	34	-4.734		103.133	1.00 74.72	Ä
	ATOM	138	CD	LYS	34	-5.218		101.986	1.00 75.69	Ä
	ATOM	139	CE	LYS	34	-6.680		101.565	1.00 75.79	A
	MOTA	140	N2	LYS	34	-7.149		101.426	1.00 74.45	A
10	MOTA	141	c	LYS	34	-5.315		102.088	1.00 70.68	A
	ATOM	142	ō	LYS	34	-6.448		101.924	1.00 70.80	A
	MOTA	143	N	ALA	35	-4.338	-1.753	101.198	1.00 68.59	A
	MOTA	144	CA	ALA	35	-4.539	-2.501	99.963	1.00 66.37	A
1.5	MOTA	145	CB	ALA	35	-3.639	~1.949	98.861	1.00 65.65	A
15	ATOM	146	С	ALA	35	-4.199		100.241	1.00 64.89	A
	MOTA	147	0	ALA	35	-4.277	-4.807	99.352	1.00 64.01	A
	ATOM	148	N	SER	36	-3.825		101.491	1.00 63.72	A
	MOTA	149	CA	SER	36	-3.454	-5.574	101.937	1.00 62.31	A
20	MOTA MOTA	150	CB	SER	36	-4.711		102.194	1.00 62.73 1.00 63.14	A A
20	ATOM	151 152	OG C	SER SER	36 36	-5.556 -2.542		100.920	1.00 60.52	A
	ATOM	153	ò	SER	36	-2.933		100.256	1.00 60.52	Ä.
	MOTA	154	N	ALA	37	-1.316	-5.759		1.00 57.81	A.
	ATOM	155	CA	ALA	37	-0.339	-6.291	99.877	1.00 54.58	A
25	ATOM	156	CB	ALA	37	0.709	-5.228	99.561	1.00 53.39	A
	ATOM	157	С	ALA	37	0.351	-7.562	100.359	1.00 51.84	A
	MOTA	158	0	ALA	37	0.586	-7.754	101.554	1.00 50.84	A
	MOTA	159	N	HIS	38	0.669	-8.429	99.405	1.00 48.60	A
20	ATOM	160	CA	HIS	38	1.363	-9.672	99.690	1.00 45.12	A
30	ATOM	161	CB	HIS	38		-10.810	98.840	1.00 48.05	A
	MOTA	162	CG	HIS	38		-10.528	97.364	1.00 50.18	A
	MOTA	163 164		HIS	38 38		-10.171	96.542 96.566	1.00 51.32 1.00 50.53	A A
	MOTA MOTA	165	ND1	HIS	38	1.875	-10.621 -10.337	95.317	1.00 50.82	A
35	MOTA	166		HIS	38	0.261		95.275	1.00 51.95	Ä
-	ATOM	167	c	HIS	38	2.836	-9.436	99.350	1.00 40.69	A
	MOTA	168	ō	HIS	38	3.165	-9.005	98.244	1.00 39.51	A
	MOTA	169	N	SER	39	3.714	-9.692	100.312	1.00 34.50	A
40	MOTA	170	CA	SER	39	5.138	-9.494	100.106	1.00 29.81	A
40	MOTA	171	CB	SER	39	5.860		101.449	1.00 29.59	A
	MOTA	172	OG	SER	39	7.263		101.265	1.00 30.93	A
	MOTA	173	C	SER	39	5.753	-10.578	99.242	1.00 27.18	A
	ATOM	174	N N	SER	39 40		-11.758	99.456 98.263	1.00 27.84 1.00 23.70	A
45	ATOM ·	175 176	ÇA	ILE	40		-10.179 -11.148	97.403	1.00 20.93	A A
•5	MOTA	177	CB	ILE	40		-10.677	95.945	1.00 21.59	Ä
	HOTA	178		ILE	40		-10.554	95.381	1.00 21.07	A
	MOTA	179		ILE	40	8.025	-9.343	95.857	1.00 21.01	A
	MOTA	180	CD1		40	8.377	-8.954	94.443	1.00 17.86	A
50	MOTA	181	С	ILE	40		-11.366	97.895	1.00 19.29	A
	MOTA	182	0	ILE	40		-12.130	97.306	1.00 18.82	A
	MOTA	183	N	VAL	41		-10.696	98.988	1.00 18.43	A
	MOTA	184	CA	VAL	41		-10.801	99.572	1.00 19.01	Α
55	MOTA MOTA	185	CB	VAL VAL	41	10.974	-9.394	99.666	1.00 18.10	A
<i>J J</i>	ATOM	186 187		VAL	41 41	12.231 11.303	-9.448 -8.881	100.525 98.279	1.00 17.03 1.00 16.81	A A
	MOTA	188	C	VAL	41		-11.420		1.00 21.10	Ä
	ATOM	189	ŏ	VAL	41		-11.122		1.00 22.16	Ä
	MOTA	190	N	GLU	42		-12.286		1.00 21.96	Ä
60	ATOM	191	CA	GLU	42		-12.894		1.00 24.43	λ
	MOTA	192	СВ	GLU	42		-14.310		1.00 26.41	A
	MOTA	193	CG	GLU	42		-14.321		1.00 33.53	A
	MOTA	194	CD	GLU	42		-15.717		1.00 37.53	A
15	MOTA	195		GLU	42		-15.830		1.00 37.91	Α
65	ATOM	196		GLU	42		-16.695		1.00 39.48	A
	MOTA	197	c	GLU	42		-12.912		1.00 23.06	A
	MOTA	198	0	GLU	42		-13.313		1.00 23.11	A
	MOTA	199	N	CYS	43		-12.461		1.00 22.56 1.00 22.27	A
70	MOTA MOTA	200 201	CA CB	CYS	43 43		-12.417 -11.032		1.00 22.27	A A
, ,	ATOM	201	SG	CYS	43	14.515		104.119	1.00 26.40	Ä
	MOTA	203	C	CYS	43		-13.458		1.00 23.32	Ä
	MOTA	204	ŏ	CYS	43		-13.850		1.00 25.24	A

	> mov	205	31	A CD	44	15 026	-13.900	105 000	1.00 24.35	A
	MOTA MOTA	205 206	N CA	ASP ASP	44		-14.897		1.00 24.49	λ
	MOTA	207	CB	ASP	44		-16.251		1.00 24.72	A
	MOTA	208	cc	ASP	44		-17.408		1.00 27.03	A
5	MOTA	209	OD1		44		-17.201		1.00 28.16	A
	MOTA	210	OD2	ASP	44	16.249	-18.531	106.780	1.00 27.08	A
	MOTA	211	С	ASP	44	17.745	-14.403	107.404	1.00 24.36	A
	MOTA	212	0	ASP	44		-14.795		1.00 23.06	A
10	MOTA	213	N	PRO	45		-13.527		1.00 25.65	Α
10	MOTA	214	CD	PRO	45		-12.911		1.00 25.98	A
	MOTA	215	ÇA	PRO	45		-12.999		1.00 26.11	· A
	MOTA	216	CB	PRO	45 45		-12.143 -11.658		1.00 25.67 1.00 26.57	A A
	ATOM	217 218	CG C	PRO PRO	45		-14.051		1.00 26.95	Ä
15	MOTA MOTA	219	Ö	PRO	45		-13.952		1.00 26.64	Ä
13	MOTA	220	N	VAL	46		-15.059		1.00 27.42	A
	ATOM	221	CA	VAL	46		-16.088		1.00 28.91	A
	MOTA	222	СВ	VAL	46		-17.105		1.00 28.55	A
	ATOM	223		VAL	46	18.882	-18.096	110.655	1.00 28.05	A
20	MOTA	224	CG2	VAL	46		-17.807		1.00 28.65	A
	MOTA	225	C	VAL	46		-16.810		1.00 30.17	A
	MOTA	226	0	VAL	46		-17.264		1.00 29.93	A
	MOTA	227	N	ARG	47		-16.893		1.00 30.73	A
25	MOTA	228	CA	ARG	47		-17.552		1.00 31.90	A A
23	MOTA	229	CB	ARG	47 47		-18.495 -19.796		1.00 35.93	A
	MOTA MOTA	230 231	CG CD	ARG ARG	47		-20.554		1.00 48.31	A
	MOTA	232	NE	ARG	47		-20.769		1.00 52.94	A
	MOTA	233	cz	ARG	47		-21.426		1.00 53.97	A
30	MOTA	234	NH1		47		-21.940		1.00 54.33	A
	MOTA	235	NH2		47		-21.561		1.00 54.58	A
	ATOM	236	С	ARG	47 .		-16.560		1.00 30.25	A
	MOTA	237	0	ARG	47	22.232	-16.965	105.122	1.00 27.99	Α
0.5	ATOM	238	N	LYS	48		-15.266		1.00 29.50	A
35	MOTA	239	CA	LYS	48		-14.228		1.00 28.39	A
	MOTA	240	CB	LYS	48		-14.362		1.00 28.24	A
	ATOM	241	CG	LYS	48		-14.762		1.00 29.13	A
	NOTA	242	CD	LYS	48		-13.656		1.00 31.53	A
40	MOTA	243	CE NZ	LYS	48 48		-13.897 -13.908		1.00 34.18	A A
70	MOTA MOTA	244 245	C	LYS	48		-14.415		1.00 37.10	À
	ATOM	246	ō	LYS	48		-14.330		1.00 27.94	A
	ATOM	247	N	GLU	49		-14.645		1.00 25.69	A
	ATOM	248	CA	GLU	49		-14.908		1.00 26.19	Ä
45	MOTA	249	CB	GŁU	49	19.300	-16.398	102.827	1.00 28.94	A
	MOTA	250	CG	GLU	49	18.711	-16.897	101.534	1.00 34.48	A
	MOTA	251	CD	GLU	49		-18.269		1.00 39.36	A
	MOTA	252		GLU	49		-18.326		1.00 40.10	A
50	MOTA	253		GLU	49		-19.285		1.00 39.93	A
30	MOTA	254	c	GLU	49		-14.113		1.00 24:38	A
	MOTA	255 256	0	GLU	49 50		-13.868 -13.715		1.00 24.72	A A
	ATOM ATOM	257	N CA	VAL	50		-12.989		1.00 22.04	Ä
	MOTA	258	CB	VAL	50		-11.553		1.00 21.63	Ä
55	MOTA	259		VAL	50		-11.619	99.127	1.00 21.68	Ä
	ATOM	260		VAL	50		-10.764		1.00 21.12	A
	ATOM	261	c	VAL	50		-13.834	99.821	1.00 19.98	A
	ATOM	262	0	VAL	50		-14.282	98.912	1.00 20.15	A
	MOTA	263	N	SER	51	15.087	-14.074	99.917	1.00 21.09	A
60	MOTA	264	CA	SER	51	14.368	-14.890	98.934	1.00 21.32	A
	ATOM	265	CB	SER	51	13.742	-16.106	99.629	1.00 20.35	A
	MOTA	266	OG	SER	51		-16.943	98.712	1.00 23.49	A
	MOTA	267	С	SER	51		-14.067	98.256	1.00 20.53	λ
65	MOTA	268	0	SER	51		-13.401	98.925	1.00 21.64	A
65	ATOM	269	N	VAL	52		-14.107	96.929	1.00 21.28	Α
	MOTA	270	CA	VAL	52		-13.348	96.189	1.00 22.46	A
	MOTA	271	CB	JAV	52		-12.293	95.282 94.605	1.00 21.66 1.00 18.69	A
	ATOM ATOM	272 273		VAL VAL	52 52		-11.462 -11.417	96.091	1.00 18.89	A
70	MOTA	274	C	VAL	52 52		-14.220	95.322	1.00 24.82	Ä
. •	MOTA	275	ο.		52		-15.099	94.597	1.00 26.25	A
	ATOM	276	N .	ARG	53		-13.964	95.409	1.00 27.28	A
	ATOM	277	CA	ARG	53		-14.690	94.638	1.00 29.70	A

	MOTA	278	CB	ARG	53	7.679	-14.562	95.341	1.00 29.44	A
	MOTA	279	CC	ARG	53		-15.238	94.658	1.00 32.62	A
•	MOTA	280	CD	ARG	53		-15.124	95.536	1.00 32.33	A
5	MOTA	281	NE	ARG	53		-15.812	96.805	1.00 34.30	A
J	HOTA	282	CZ	ARG	53		-15.618	97.894	1.00 35.73	A
	ATOM	283 284		ARG ARG	53 53		-14.743 -16.297	97.877 99.001	1.00 35.26 1.00 33.24	A A
	MOTA MOTA	285	C	ARG	53		-14.062	93.243	1.00 30.22	Ä
	ATOM	286	ŏ	ARG	53		-12.922	93.080	1.00 28.70	A
10	MOTA	287	N	THR	54		-14.809	92.244	1.00 32.13	Ä
	ATOM	288	CA	THR	54		-14.314	90.872	1.00 35.09	A
	ATOM	289	CB	THR	54		-14.788	90.153	1.00 34.03	A
	MOTA	290		THR	54		-16.218	90.086	1.00 33.22	A
	MOTA	291	CG2	THR	54	12.026	-14,305	90.898	1.00 33.36	A
15	MOTA	292	С	THR	54		-14.705	90.011	1.00 38.38	A
	MOTA	293	0	THR	54		-14.098	BB.970	1.00 39.08	λ
	MOTA	294	N	GLY	55		-15.717	90.435	1.00 42.35	A
	MOTA	295	CA	GLY	55		-16.145	89.653 90.171	1.00 47.68 1.00 52.55	A A
20	MOTA MOTA	296 297	0	GLY	55 55		-15.562 -14.562	89.651	1.00 52.62	Ä
20	ATOM	298	N	GLY	56		-16.196	91.204	1.00 56.07	Ä
	ATOM	299	CA	GLY	56		-15.734	91.789	1.00 58.64	A.
	MOTA	300	c c	GLY	56		-16.804	92.620	1.00 60.65	A
	MOTA	301	Ó	GLY	56		-17.999	92.444	1.00 60.57	A
25	MOTA	302	N	LEU	57	1.795	-16.364	93.532	1.00 62.43	A
	MOTA	303	CA	LEU	57		-17.253	94.421	1.00 63.41	A
	MOTA	304	CB	LEU	57		-18.425	93.627	1.00 63.91	A
	MOTA	305	CG	LEU	57		-18.152	92.419	1.00 64.67	A
30	MOTA	306		LEU	57		-19.486	91.873	1.00 64.88	Α.
30	ATOM	307		LEU	57		-17.276	92.806	1.00 64.92 1.00 63.25	A
	MOTA	308 309	C	LEU	57 57		-17.800 -18.393	95.586 95.383	1.00 63.23	A A
	MOTA MOTA	310	O N	ALA	58		-17.591	96.807	1.00 62.63	A
	MOTA	311	CA	ALA	58		-18.074	98.010	1.00 61.38	A
35		. 312	СВ	ALA	58		-17.286	99.229	1.00 60.84	A
	MOTA	313	c	ALA	58		-19.562	98.184	1.00 60.68	A
	MOTA	314	0	ALA	58		-20.261	98.979	1.00 60.38	A
	ATOM	315	N	ASP	59		-20.024	97.422	1.00 59.38	A
40	MOTA	316	CA	ASP	59		-21.413	97.427	1.00 57.30	A
40	MOTA	317	СВ	ASP	59		-21.498	96.770	1.00 58.25	A
	MOTA	318	CG	ASP	59		-22.907	96.386	1.00 58.65	A
	ATOM	319		ASP	59 50		-23.767	97.285	1.00 58.25	A A
	MOTA MOTA	320 321	C C	ASP ASP	59 59		-23.151 -22.267	95.175 96.652	1.00 55.60	A
45	ATOM	322	ò	ASP	59		-23.414	97.007	1.00 55.05	Â
	MOTA	323	N	LYS	60		-21.681	95.587	1.00 53.85	A
	ATOM	324	CA	LYS	60		-22.340	94.718	1.00 51.83	A
	MOTA	325	CB	LYS	60		-23.322	93.787	1.00 52.01	A
	MOTA	326	CG	LYS	60	2.982	-23.940	92.720	1.00 51.22	A
50	ATOM	327	CD	LYS	60		-24.835	91.795	1.00 50.89	A
	HOTA	328	CE	LYS	60		-25.341	90.663	1.00 52.06	A
	MOTA	329	NZ	LYS	60		-24.213	89.891	1.00 52.67	A
	ATOM	330 331	c	LYS	60		-21.258	93.900	1.00 50.64	A
55	MOTA	332	0	LYS SER	60 61		-20.350 -21.347	93.358 93.805	1.00 51.26	A A
JJ	MOTA MOTA	333	N CA	SER	61		-20.340	93.056	1.00 42.61	Ä
	MOTA	334	CB	SER	61		-18.996	93.778	1.00 42.79	A
	ATOM	335	OG	SER	61		-19.048	95.039	1.00 41.39	A
	MOTA	336	c	SER	61		-20.668	92.846	1.00 40.50	A
60	ATOM	337	0	SER	61		-21.619	93.412	1.00 39.84	A
	MOTA	338	N	SER	62		-19.856	92.017	1.00 37.70	A
	MOTA	339	ÇA	SER	62		-19.998	91.732	1.00 34.42	A
	MOTA	340	CB	SER	62		-19.776	90.245	1.00 34.68	A
65	ATOM	341	OG	SER	62		-19.881	89.964	1.00 38.74	A
65	ATOM	342	C	SER	62		-18.917	92.554	1.00 32.09	A
	HOTA	343	0	SER	62		-17.903	92.888	1.00 29.47	A
	MOTA	344 345	И	ARG ARG	63 63		-19.126 -18.136	92.896 93.690	1.00 30.00	A A
	ATOM ATOM	345	CA CB	ARG	63		-18.472	95.189	1.00 29.48	A
70	ATOM	347	CG	ARG	63		-18.695	95.710	1.00 35.27	Ä
. •	HOTA	348	CD	ARG	63		-18.504	97.218	1.00 37.21	A
	ATOM	349	NE	ARG	63		-17.093	97.590	1.00 42.67	A
	MOTA	350	CZ	ARG	63		-16.601	98.768	1.00 44.05	A

	» mov	251			63	0 005	15 200	00 014	1.00 42.72	
	MOTA MOTA	351 352	NH1		63 63		-15.299	99.014 99.700	1.00 46.01	A A
	ATOM	353	NH2 C	ARG	63		-17.408 -17.994	93.314	1.00 27.46	Ä
	ATOM	354	ō	ARG	63		-18.887	92.702	1.00 26.59	Ä
5	MOTA	355	N	LYS	64		-16.853	93.693	1.00 25.59	A
-	ATOM	356	CA	LYS	64		-16.539	93.467	1.00 23.77	A
	ATOM	357	СВ	LYS	64		-15.299	92.587	1.00 25.43	A
	MOTA	358	CG	LYS	64		-15.532	91.231	1.00 26.32	A
	ATOM	359	ന	LYS	64	15.095	-16.338	90.323	1.00 28.26	A
10	MOTA	360	CE	LYS	64	15.692	-16.456	88.925	1.00 29.50	A
	MOTA	361	NZ	LYS	64	15.825	-15.135	88.250	1.00 27.38	A
	MOTA	362	С	LYS	64		-16.257	94.854	1.00 23.10	Α
	MOTA	363	0	LYS	64		-15.488	95.637	1.00 22.42	A
15	ATOM	364	N	THR	65		-16.876	95.154	1.00 22.03	A
15	ATOM	365	CA	THR	65		-16.715	96.452	1.00 20.67	A
	MOTA	366	CB	THR	65		-18.081	97.179	1.00 21.12	A
	MOTA MOTA	367	0G1		65		-18.252 -18.187	97.870 98.154	1.00 22.06 1.00 27.20	A A
	ATOM	368 369	CG2 C	THR	65 65		-16.136	96.363	1.00 19.65	A
20	ATOM	370	ō	THR	65	19.735	-16.430	95.425	1.00 22.34	Ä
	ATOM	371	N	TYR	- 66		-15.300	97.331	1.00 17.01	A
	ATOM	372	CA	TYR	66		-14.695	97.349	1.00 15.46	A
	ATOM	373	CB	TYR	66		-13.244	96.829	1.00 14.31	A
	ATOM	374	CG	TYR	66	20.034	-13.055	95.482	1.00 14.28	A
25	MOTA	375	CD1	TYR	66	18.651	-12.984	95.366	1.00 12.32	A
	MOTA	376	CEl	TYR	66		-12.799	94.130	1.00 14.42	A
	ATOM	377	CD2	TYR	66		-12.938	94.320	1.00 12.69	A
	ATOM	378		TYR	66	20.207	-12.752	93.079	1.00 10.53	A
20	ATOM	379	CZ	TYR	66	18.829	-12.682	92.993	1.00 13.34	A
30	MOTA	380	ОН	TYR	66		-12.483	91.776	1.00 14.95	A
	MOTA	381	C	TYR	66		-14.675	98.754	1.00 14.50 1.00 13.73	A A
	MOTA MOTA	382	о И	TYR	66 67		-14.461 -14.880	99.733 98.854	1.00 14.35	A
	MOTA	383 384	CA	THR	67	23.260	-14.853		1.00 15.82	Ä
35	MOTA	385	CB	THR	67		-16.127		1.00 16.72	A
	MOTA	386	0G1		67		-17.261		1.00 17.16	A
	MOTA	387	CG2		67			101.698	1.00 17.80	A
	MOTA	388	С	THR	67		-13.650		1.00 16.72	A
	MOTA	389	0	THR	67	24.992	-13.450	99.293	1.00 17.55	A
40	ATOM	390	N	PHE	68		-12.839		1.00 16.84	A
	MOTA	391	CA	PHE	68		-11.666		1.00 18.85	, A
	MOTA	392	СВ	PHE	68		-10.371		1.00 17.59	Α
	MOTA	393	CC	PHE	68		-10.206		1.00 17.32	A
45	MOTA	394	CD1		68		-10.823 -9.447	99.926 99.036	1.00 16.89 1.00 17.68	A A
73	MOTA MOTA	395 396	CD2 CE1		68 68	23.855 21.387	-10.680	98.752	1.00 17.00	Ä
	ATOM	397	CE2		68	23.144	-9.296	97.852	1.00 16.89	Ä
	MOTA	398	cz	PHE	68	21.906	-9.916	97.708	1.00 17.47	A
	MOTA	399	c	PHE	68		-11.731		1.00 19.38	A
50	MOTA	400	0	PHE	68	25.505	-12.703	103.479	1.00 21.74	A
	MOTA	401	N	ASP	69	26.388	-10.688	103.078	1.00 19.56	A
	MOTA	402	CA	ASP	69	27.105	-10.670		1.00 20.30	A
	MOTA	403	CB	ASP	69	28.177		104.313	1.00 20.07	A
55	MOTA	404	CG	ASP	. 69	29.306		103.332	1.00 22.41	λ
دد	MOTA	405	OD1	ASP	. 69	29.245		102.143	1.00 20.37	A
	MOTA	406	OD2	ASP	69		-10.582 -10.500		1.00 27.46	A A
	MOTA MOTA	407 408	С 0	ASP ASP	69 69		-11.073		1.00 20.33	Ä
	ATOM	409	N	MET	70	25.091		105.325	1.00 21.04	Ä
60	MOTA	410	CA	MET	70	24.065		106.338	1.00 20.59	A
••	MOTA	411	CB	MET	70	24.464		107.257	1.00 23.87	A
	ATOM	412	CG	MET	70	25.600		108.202	1.00 27.55	A
	MOTA	413	SD	MET	70	25.794		109.420	1.00 28.63	A
	MOTA	414	CE	MET	70	24.665		110.676	1.00 29.22	A
65	MOTA	415	С	MET	70	22.737		105.678	1.00 20.50	A
	ATOM	416	0	MET	70	22.697		104.657	1.00 19.82	A
	MOTA	417	И	VAL	71	21.646		106.258	1.00 18.11	A
	ATOM	418	CA	VAL	71	20.335		105.713	1.00 17.48	A
70	ATOM	419	CB	VAL	71		-10.516		1.00 17.16	A
70	ATOM	420	CG1		71		-10.915		1.00 14.56	A
	ATOM ATOM	421 422	CG2		71 71	19.625	-11.662	105.986	1.00 19.68 1.00 16.09	A A
•	ATOM	423	C O	VAL VAL	71	19.424		100.022	1.00 14.72	Ä
	A. JE	763	•	1110	• •		٠.٠.٥		1.00 142	^

	ATOM	424	N	PHE	72	18.714	-7.706 106.529	1.00 16.25	A
	ATOM	425	CA	PHE	72	17.793	-7.075 107.460	1.00 15.53	A
	ATOM	426	CB	PHE	72	18.289	-5.670 107.799	1.00 14.92	A
						19.575	-5.658 108.575	1.00 17.03	
5	ATOM	427	CC	PHE	72				A
J	MOTA	428	CD1		72	19.590	-6.004 109.925	1.00 16.20	A
	MOTA	429	CD2	PHE	72	20.782	-5.332 107.950	1.00 17.34	A
	ATOM	430	CE1	PHE	72	20.785	-6.026 110.649	1.00 16.42	A
	ATOM	431	CE2	PHÉ	72	21.979	-5.352 108.660	1.00 16.87	A
	MOTA	432	CZ	PHE	72	21.983	-5.702 110.016	1.00 16.79	A
10	MOTA				72	16.388	-7.007 106.874	1.00 15.43	A
10		433	С	PHE					
	MOTA	.434	0	PHE	72	16.163	-6.394 105.834	1.00 13.98	A
	ATOM	435	N	GLY	73	15.445	-7.646 107.557	1.00 18.08	A
	MOTA	436	CA	GLY	73	14.067	-7.655 107.104	1.00 17.75	A
	MOTA	437	С	GLY	73	13.343	-6.377 107.478	1.00 19.38	A
15	ATOM	438		GLY	73	13.918	-5.477 108.101	1.00 19.14	A
	ATOM	439		ALA	74	12.069	-6.308 107.103	1.00 20.07	A
							-5.145 107.363		
	MOTA	440	CA	ALA	74	11.228		1.00 20.00	A
	MOTA	441	CB	ALA	74	9.840	-5.399 106.800	1.00 19.61	A
	MOTA	442	С	ALA	74	11.124	-4.709 108.834	1.00 19.69	A
20	MOTA	443	0	ALA	74	10.972	-3.525 109.123	1.00 21.06	Α
	MOTA	444	N	SER	75	11.213	-5.650 109.765	1.00 18.30	A
	ATOM	445	CA	5ER	75	11.103	-5.300 111.177	1.00 18.31	A
	MOTA		CB	SER	75			1.00 16.40	Α.
		446				10.789	-6.553 111.991		
25	MOTA	447		SER	75	11.886	-7.450 111.971	1.00 15.90	A
25	MOTA	448	С	SER	75	12.359	-4.625 111.748	1.00 18.96	A
	MOTA	449	0	SER	75	12.368	-4.196 112.902	1.00 19.99	A
	MOTA	450	N	THR	76	13.407	-4.519 110.937	1.00 18.45	A
	ATOM	451	CA	THR	76	14.567	-3.932 111.390	1.00 17.88	A
	ATOM	452		THR	76	15.783	-4.165 110.347	1.00 18.01	A
30	ATOM	453	0G1		76	15.861	-5.567 110.019	1.00 17.20	A
20									
	ATOM	454	CG2		76	17.109	-3.708 110.902	1.00 17.48	A
	MOTA	455		THR	76	14.570	-2.437 111.687	1.00 17.40	A
	MOTA	456	0	THR	76	14.064	-1.667 110.877	1.00 18.84	A
	ATOM	457	N	LYS	77	15.061	-2.034 112.853	1.00 16.09	A
35	MOTA	458		LYS	77	15.032	-0.633 113.262	1.00 17.09	Α
	MOTA	459		LYS	77	14.667	-0.526 114.751	1.00 19.20	A
					77	13.337			A
	MOTA	460		LYS			-1.181 115.120	1.00 20.20	
	ATOM	461		LYS	77	12.198	-0.604 114.302	1.00 24.17	A
40	MOTA	462		LYS	7 7	10.882	-1.325 114.556	1.00 28.56	A
40	ATOM	463	NZ	LYS	77	9.741	-0.673 113.832	1.00 29.29	A
	MOTA	464	С	LYS	77	16.383	0.039 113.007	1.00 16.81	A
	ATOM	465	0	LYS	77	17.382	-0.638 112.760	1.00 16.91	A
	ATOM	466	N	GLN	78	16.414	1.368 113.067	1.00 14.39	A
	MOTA	467		GLN	78	17.657	2.101 112.831	1.00 13.21	A
45									
47	MOTA	46B		GLN	78	17.422	3.611 112.945	1.00 10.26	A
	MOTA	469		GLN	78	16.343	4.179 112.017	1.00 10.24	· A
	MOTA	470	CD	GLN	78	16.799	4.325 110.579	1.00 8.85	A
	MOTA	471	OE1	GLN	78	17.170	3.348 109.922	1.00 10.32	A
	MOTA	472	NE2	GLN	78	16.776	5.555 110.081	1.00 6.58	A
50	ATOM	473	С	GLN	78	18.750	1.687 113.821	1.00 13.02	A
	ATOM	474		GLN	78	19.933	1.636 113.474	1.00 11.38	Ä
	ATOM	475		ILE	79	18.352	1.392 115.053	1.00 12.89	Ä
	MOTA	476		ILE	79	19.313	1.013 116.085	1.00 13.42	A
	MOTA	477		ILE	79	18.635	0.959 117.479	1.00 13.40	A
55	ATOM	.478	CG2	ILE	79	17.591	-0.142 117.508	1.00 14.83	A
	MOTA	479	CG1	ILE	79	19.684	0.733 118.571	1.00 13.65	A
	MOTA	480	CD1	ILE	79	20.653	1.906 118.775	1.00 14.47	A
	ATOM	481		ILE	79	19.972	-0.329 115.771	1.00 12.91	A
	ATOM	482		ILE	79	21.157	-0.522 116.044	1.00 12.01	A
60									
00	MOTA	483	N	ASP	80	19:204	-1.243 115.182	1.00 13.40	A
	ATOM	484		ASP	80	19.719	-2.555 114.815	1.00 14.93	A
	MOTA	485	CB	ASP	80	18.581	-3.461 114.303	1.00 17.57	λ
	ATOM	486	CG	ASP	80	17.428	-3.593 115.300	1.00 20.41	A
	ATOM	487	OD1	ASP	80	17.692	-3.811 116.504	1.00 22.08	A
65	ATOM	488	OD2		80	16.253	-3.492 114.879	1.00 21.37	A
-	MOTA	489		ASP			-2.393 113.719		
					80	20.777		1.00 15.46	λ
	MOTA	490		ASP	80	21.845	-3.007 113.769	1.00 15.07	A
	MOTA	491		VAL	81	20.467	-1.560 112.730	1.00 15.97	A
	MOTA	492	CA	VAL	81	21.380	-1.307 111.625	1.00 16.25	A
70	MOTA	493	CB	VAL	81	20.747	-0.360 110.555	1.00 16.07	A
	MOTA	494	CG1		81	21.787	0.027 109.526	1.00 14.56	Α
	ATOM	495	CG2		81	19.568	-1.049 109.857	1.00 14.48	A
		496		VAL	81			1.00 14.48	À
	MOTA	430	_	* AL	04	22.667	-0.681 112.142	1.00 10.37	^

	ATOM	497	0	VAL	81	23.758	-1.079	111.733	1.00 20.96	A
	MOTA	498	N	TYR	82	22.549	0.289	113.046	1.00 19.05	A
	MOTA	499	CA	TYR	82	23.732		113.583	1.00 20.41	A
	ATOM	500	CB	TYR	82	23.339		114.471	1.00 23.17	A
5.	ATOM	501	CG	TYR	82				1.00 24.73	A
,						24.532		114.992		
	MOTA	502		TYR	82	25.137		116.198	1.00 24.58	A
	MOTA	503	CE1		82	26.284		116.638	1.00 25.15	A
	ATOM	504	CD2	TYR	82	25.107	3.928	114.237	1.00 25.38	A
_	MOTA	505	CE2	TYR	82	26.258	4.576	114.668	1.00 25.61	A
10	ATOM	506	cz	TYR	82	26.842	4.204	115.868	1.00 25.89	A
	MOTA	507	OH	TYR	82	28.000		116.297	1.00 26.74	A
		508								A
	MOTA		C	TYR	82	24.633		114.375	1.00 22.16	
	MOTA	509	0	TYR	82	25.835		114.103	1.00 22.17	A
	MOTA	510	N	ARG	83	24.059	-0.694	115.352	1.00 21.11	A
15	ATOM	511	CA	ARG	83	24.834	-1.615	116.170	1.00 20.40	A
	MOTA	512	CB	ARG	83	23.928	-2.263	117.222	1.00 18.85	A
	ATOM	513	CG	ARG	83	23.521		118.339	1.00 21.14	A
	MOTA	514	CD	ARG	83	22.272		119.065	1.00 21.88	A
	ATOM	515	NE	ARG	83	22.478		119.779	1.00 22.27	A
20										
20	MOTA	516	CZ	ARG	83	23.184		120.899	1.00 23.18	A
	ATOM	517		ARG	83	23.757		121.434	1.00 23.11	A
	MOTA	518	NH2	ARG	83	23.30B	-4.356	121.490	1.00 23.57	A
	ATOM	519	С	ARG	83	25.553	-2.694	115.361	1.00 19.49	A
	MOTA	520	0	ARG	83	26.702	-3.022	115.647	1.00 17.49	A
25	MOTA	521	N	SER	84	24.885		114.341	1.00 19.74	. A
	ATOM	522	CA	SER	84	25.462		113.519	1.00 19.67	A
	ATOM	523	CB	SER	84			112.888	1.00 21.49	A
						24.359				
	MOTA	524	OG	SER	84	23.716		113.865	1.00 28.64	Α
20	MOTA	525	С	SER	84	26.419		112.426	1.00 18.56	A
30	MOTA	526	0	SER	84	27.487	-4.436	112.302	1.00 19.77	A
	ATOM	527	N	VAL	85	26.058	-2.866	111.624	1.00 18.63	A
	ATOM	528	CA	VAL	85	26.949	-2.470	110.542	1.00 19.52	A
	MOTA	529	CB	VAL	85	26.161		109.222	1.00 19.26	A
	ATOM	530		VAL	85	25.165		109.011	1.00 20.45	A
35				VAL						
33	MOTA	531			85	25.448		109.251	1.00 22.19	A
	ATOM	532	С	VAL	85	27.828		110.810	1.00 19.41	A
	MOTA	533	0	VAL	85	29.034	-1.289	110.558	1.00 19.81	A
	ATOM	534	N	VAL	86	27.236	-0.189	111.342	1.00 19.42	A
	MOTA	535	CA	VAL	86	27.959	1.053	111.603	1.00 19.60	A
40	ATOM	536	CB	VAL	86	26.971		111.815	1.00 18.59	A
. •	ATOM	537		VAL	86	27.724		111.800	1.00 19.00	A
	MOTA	538	CG2						1.00 18.56	A
					86	25.899		110.736		
	MOTA	539	C	VAL	86	28.950		112.773	1.00 20.31	λ
45	MOTA	540	0	VAL	86	30.060		112.637	1.00 19.36	A
45	MOTA	541	N	CYS	87	28.559	0.519	113.919	1.00 21.30	A
	MOTA	542	CA	CYS	87	29.438	0.535	115.082	1.00 23.03	A
	ATOM	543	CB	CYS	87	28.777	-0.187	116.254	1.00 26.09	A
	-MOTA	544	SG	CYS	87	29.481		117.859	1.00 36.72	A
	MOTA	545	c	CYS	87	30.824		114.804	1.00 21.77	A
50	MOTA	546	ŏ	CYS	87	31.835		115.145	1.00 21.30	Ä
50										
	MOTA	547	N	PRO	88	30.894		114.185	1.00 20.49	Α
	ATOM	548	CD	PRO	88	29.856		113.881	1.00 20.97	A
	MOTA	549	CA	PRO	88	32.231	-1.783	113.926	1.00 20.97	A
	ATOM	550	CB	PRO	88	31.948	-3.215	113.473	1.00 18.41	A
55	MOTA	551	CG	PRO	88	30.571	-3.133	112.895	1.00 20.02	A
	MOTA	552	C	PRO	88	33.052		112.905	1.00 21.87	A
	ATOM	553	ō	PRO	88	34.280		113.000	1.00 22.69	A
		554	N		89			111.934	1.00 21.27	A
	MOTA			ILE		32.380				
40	ATOM	555	CA	ILE	89	33.068		110.915	1.00 20.39	A
60	ATOM	556	CB	ILE	89	32.130	0.723	109.720	1.00 20.42	A
	MOTA	557	CG2	ILE	89	32.791	1.710	108.762	1.00 16.94	A
	MOTA	558	CG1	ILE	89	31.786	-0.584	108.998	1.00 20.17	A
	MOTA	559		ILE	89	30.749		107.886	1.00 21.44	A
	ATOM	560	c	ILE	89	33.577		111.515	1.00 21.10	A
65										
U J	MOTA	561	0	ILE	89	34.640		111.144		A
	MOTA	562	N	LEU	90	32.818		112.449	1.00 20.96	A
	MOTA	563	CA	LEU	90	33.229		113.103	1.00 20.72	A
	MOTA	564	CB	LEU	90	32.086	4.094	113.940	1.00 18.19	A
	ATOM	565	CG	LEU	90	32.407	5.390	114.687	1.00 19.36	A
70	MOTA	566		LEU	90	32.779		113.702	1.00 17.91	A
. •	MOTA	567		LEU	90	31.203		115.515	1.00 19.74	A
									1.00 19.74	
	MOTA	568	C	LEU	90	34.443		113.989		A
	MOTA	569	0	LEU	90	35.346	4.081	114.089	1.00 22.10	A

	ATOM	570	N	ASP	91	34.471	2.084 1	14 632	1.00	21.61	A
		571							1.00		
	MOTA		CA	ASP	91	35.611	1.731 1				A
	MOTA	572	CB	ASP	91	35.404	0.380 1		1.00		A
_	MOTA	573	CG	ASP	91	34.535	0.486 1	17.410	1.00	25.39	A
5	MOTA	574	ODl	ASP	91	34.386	1.604 1	17.947	1.00	24.95	A
	MOTA	575	OD2	ASP	91	34.006	-0.552 1		1.00	27.30	A
	ATOM	576	c	ASP	91	36.877	1.667 1		1.00		A
	MOTA										
		577	0	ASP	91	37.956	2.039 1		1.00		A
10	ATOM	578	N	GLU	92	36.749	1.199 1		1.00		A
10	MOTA	579	CA	GLU	92	37.907	1.130 1	.12.499	1.00	22.88	A
	MOTA	580	CB	GLU	92	37.599	0.311 1	11.238	1.00	24.90	A
	ATOM	581	CG	GLU	92	38.131	-1.120 1		1.00		A
	ATOM	582	CD	GLU	92	38.517	-1.655 1		1.00		A
15	ATOM	583		GLU	92	39.330	-1.007 1		1.00		A
15	MOTA	584	OE2	GLU	92	38.017	-2.732 1		1.00		A
	ATOM	585	С	GLU	92	38.358	2.537 1	12.100	1.00	22.24	A
	MOTA	586	0	GLU	92	39.554	2.799 1	11.964	1.00	21.80	A
	ATOM	587	N	VAL	93	37.398	3.438 1		1.00	20.21	A
	ATOM	588	CA	VAL	93	37.712	4.808 1		1.00		A
20											
20	MOTA	589	CB	VAL	93	36.422	5.626 1		1.00		A
	MOTA	590		VAL	93	36.755	7.102 1		1.00		A
	ATOM	591	CG2	VAL	93	35.781	5.124 1	.09.937	1.00	16.29	Α.
	ATOM	592	С	VAL	93	38.489	5.482 1	12.657	1.00	19.09	A
	MOTA	593	0	VAL	93	39.477	6.174 1	12.414	1.00	18.02	A
25	MOTA	594	N	ILE	94	38.044	5.263 1		1.00		A
									1.00		
	MOTA	595	CA	ILE	94	38.690	5.845 1				A
	MOTA	596	CB	ILE	94	37.815	5.615 1		1.00		A
	MOTA	597	CG2	ILE	94	38.519	6.128 1	.17.571	1.00		A
	MOTA	598	CG1	ILE	94	36.472	6.336 1	16.124	1.00	22.49	A
30	MOTA	599	CD1	ILE	94	35.480	6.155 1	17.266	1.00	22.50	Α
	ATOM	600	c	ILE	94	40.116	5.302 1		1.00		A
											A
	MOTA	601	0	ILE	94	40.924	5.931 1		1.00		
	ATOM	602	N	MET	95	40.428	4.148 1	-	1.00		A
25	MOTA	603	CA	MET	95	41.767	3.559 1		1.00		A
35	ATOM	604	CB	MET	95	41.732	2.047 1	14.532	1.00	29.33	A
	MOTA	605	CG	MET	95	41.102	1.237 1	15.643	1.00	35.68	A
	MOTA	606	SD	MET	95	41.281	-0.526 1	15.337	1.00	44.01	A
	MOTA	607	CE	MET	95	39.718	-0.911 1		1.00		A
		608		MET					1.00		Ä
40	MOTA		c		95	42.722	4.183 1				
40	MOTA	609	0	MET	95	43.907	3.832 1		1.00		A
	MOTA	610	N	GLY	96	42.197	5.088 1		1.00		A
	MOTA.	611	CA	GLY	96	43.020	5.753 1	11.941	1.00	26.52	A
	ATOM	612	С	GLY	96	42.861	5.220 1	10.529	1.00	25.69	A
	ATOM	613	0	GLY	96	43.752	5.373 1		1.00		A
45	ATOM	614	N	TYR	97	41.720	4.597 1		1.00		Α
											A
	MOTA	615	CA	TYR	97	41.439	4.033 1		1.00		
	ATOM	616	CB	TYR	97	40.932	2.592 1		1.00		A
	ATOM	617	CC	TYR	97	42.007	1.569 1		1.00		A
~~	ATOM	618	CD1	TYR	97	42.993	1.243 1	.08.514	1.00	36.66	A
50	MOTA	619	CEl	TYR	97	43.970	0.292 1	08.798	1.00	39.73	A
	MOTA	620	CD2	TYR	97	42.025	0.914 1	10.680	1.00	35.77	A
	ATOM	621	CE2		97	42.998	-0.037 1		1.00		A
		622			97		-0.342 1		1.00		A
	ATOM		CZ	TYR		43.969					
E E	MOTA	623	ОН	TYR	97	44.956	-1.264 1		1.00		A
55	MOTA	624	С	TYR	97	40.407	4.854 1	.08.163	1.00	22.65	A
	MOTA	625	0	TYR	97	39.749	5.741 1	08.711	1.00	22.45	A
	ATOM	626	- N	ASN	98	40.290	4.565 1	06.872	1.00	19.89	A
	ATOM	627	CA	ASN	98	39.312	5.226 1		1.00		A
	MOTA	628	CB	ASN	98	39.941	5.682 1		1.00		A
60											
UU	MOTA	629	CG	ASN	98	40.867	6.863 1		1.00		A
	ATOM	630	ODl	ASN	98	40.543	7.826 1	.05.574	1.00		A
	ATOM	631	ND2	ASN	98	42.020	6.807 1	04.222	1.00	20.02	A
	ATOM	632	С	ASN	98	38.195	4.230 1		1.00	18.68	A
	MOTA	633	õ	ASN	98	38.459	3.087 1		1.00		A
65									1.00		
UJ	MOTA	634	N	CYS	99	36.949	4.657 1				A
	MOTA	635	CA	CYS	99	35.825	3.776 1		1.00		A
	MOTA	636	CB	CYS	99	35.244	3.186 1	06.867	1.00	18.42	Α
	ATOM	637	SG	CYS	99	36.378	2.095 1	07.771	1.00	19.49	A
	ATOM	638	c	CYS	99	34.727	4.481 1		1.00		A
70	ATOM	639	ō	CYS	99	34.508	5.685 1		1.00		Ä
. •											
	MOTA	640	N	THR	100	34.044	3.696 1		1.00		A
	MOTA	641	CA	THR	100	32.968	4.190 1		1.00		A
	ATOM	642	CB	THR	100	33.417	4.278 1	01.657	1.00	12.78	A

	MOTA	643	OG1	THE	100	34.485	5 223	101.539	1.00 14.13	A
	MOTA	644		THR	100	32.262				
								100.773	1.00 12.44	A
	MOTA	645		THR	100	31.759		103.200	1.00 14.15	A
-	MOTA	646	0	THR	100	31.907		103.263	1.00 13.80	A
5	ATOM	647	N	ILE	101	30.568	3.851	103.199	1.00 12.37	A
	MOTA	648	CA	ILE	101	29.329	3.088	103.202	1.00 11.07	A
	ATOM	649		ILE	101	28.608		104.551	1.00 10.99	A
		650	CG2		101			104.527		
	MOTA					27.404			1.00 11.07	A
10	MOTA	651	CG1		101	29.551		105.682	1.00 11.36	A
10	ATOM	652	CD1	ILE	101	28.880	2.767	107.071	1.00 11.31	A
	MOTA	653	С	ILE	101	28.394	3.659	102.123	1.00 10.34	A
	ATOM	654		ILE	101	28.077		102.133	1.00 8.62	A
	ATOM	655		PHE	102	27.980		101.192	1.00 8.88	Α
16	MOTA	656		PHE	102	27.089		100.113	1.00 8.18	A
15	ATOM	657	CB	PHE	102	27.521	2.554	98.798	1.00 8.39	A
	ATOM	658	CG	PHE	102	28.786	3.107	98.212	1.00 8.44	A
	MOTA	659	CD1	PHE	102	28.746	4.237	97.400	1.00 8.21	A
	MOTA	660	CD2		102	30.004	2.449	98.402	1.00 7.42	A
							4.712			Ä
20	MOTA	661	CE1		102	29.901		96.770	1.00 10.64	
20	MOTA	662	CE2		102	31.167	2.910	97.780	1.00 9.88	A
	ATOM	663	CZ	PHE	102	31.119	4.044	96.957	1.00 10.26	A
	MOTA	664	С	PHE	102	25.686	2.695	100.418	1.00 9.34	Α
	ATOM	665		PHE	102	25.514	1.676	101.084	1.00 9.83	A
	MOTA	666		ALA	103	24.686	3.420	99.937	1.00 8.83	A
25										
23	ATOM	667		ALA	103	23.301		100.088	1.00 6.41	Α
	ATOM	668		ALA	103	22.503		100.836	1.00 6.59	A
	MOTA	669	С	ALA	103	22.887	2.920	98.619	1.00 5.06	A
	MOTA	670	0	ALA	103	22.988	3.898	97.890	1.00 3.08	A
	MOTA	671	N	TYR	104	22.476	1.735	98.184	1.00 4.26	A
30	ATOM	672		TYR	104	22.110	1.498	96.791	1.00 4.91	A
50	ATOM	673		TYR	104		0.552	96.137		A
						23.142				
	MOTA	674		TYR	104	22.911	0.238	94.666	1.00 4.19	A
	MOTA	675	CD1	TYR	104	21.933	-0.675	94.260	1.00 6.04	A
	ATOM	676	CE1	TYR	104	21.722	-0.946	92.898	1.00 7.93	A
35	ATOM	677	CD2	TYR	104	23.667	0.868	93.679	1.00 5.77	A
	ATOM	678	CE2		104	23.466	0.608	92.326	1.00 5.74	A
	MOTA	679		TYR	104	22.500	-0.295	91.944	1.00 6.93	A
	ATOM	680		TYR	104	22.326	-0.551	90.604	1.00 8.61	A
40	MOTA	681	C	TYR	104	20.718	0.893	96.678	1.00 5.23	A
40	MOTA	682	0	TYR	104	20.346	0.007	97.445	1.00 7.02	A
	ATOM	683	N	GLY	105	19.955	1.368	95.704	1.00 3.82	A
	MOTA	684		GLY	105	18.620	0.857	95.521	1.00 5.02	A
	MOTA	685		GLY	105	17.705	1.803	94.773	1.00 5.87	A
45	MOTA	686		GLY	105	17.981	2.992	94.590	1.00 6.06	A
43	MOTA	687		GLN	106	16.598	1.244	94.326	1.00 4.13	A
	ATOM	688	CA	GLN	106	15.601	1.986	93.591	1.00 6.44	A
	MOTA	689	CB	GLN	106	14.513	0.998	93.158	1.00 6.41	Α
	ATOM	690	CG	GLN	106	13.175	1.585	92.817	1.00 11.96	Α
	ATOM	691	CD	GLN	106	12.136	0.511	92.499	1.00 14.57	A
50	MOTA	692	OE1		106	12.060	-0.539	93.172	1.00 12.16	A
-	ATOM	693		GLN	106	11.318	0.774	91.483		Ä
									1.00 10.80	
	MOTA	694		GLN	106	15.047	3.091	94.488	1.00 7.89	A
	MOTA	695		GLN	106	15.083	2.992	95.725	1.00 8.30	A
	MOTA	696	N	THR	107	14.558	4.157	93.869	1.00 8.49	A
55	MOTA	697	CA	THR	107	13.981	5.259	94.620	1.00 8.83	A
	MOTA	698		THR	107	13.532	6.371	93.668	1.00 10.17	A
	ATOM	699	OG1		107	14.681	6.936	93.023	1.00 11.92	A
	ATOM	700		THR	107	12.783	7.464	94.431	1.00 9.05	A
~	MOTA	701		THR	107	12.763	4.751	95.392	1.00 11.60	A
60	MOTA	702	0	THR	107	11.936	4.017	94.838	1.00 13.74	A
	ATOM	703	N	GLY	108	12.661	5.121	96.668	1.00 11.74	A
	ATOM	704		GLY	108	11.527	4.703	97.476	1.00 9.99	A
	ATOM	705		GLY	108	11.738	3.461	98.330	1.00 11.25	Ä
65	MOTA	706		GLY	108	10.812	3.004	99.018	1.00 12.52	A
υJ	MOTA	707		THR	109	12.947	2.915	98.313	1.00 9.04	A
	MOTA	708	CA	THR	109	13.216	1.716	99.090	1.00 8.13	A
	MOTA	709	CB	THR	109	14.053	0.703	98.291	1.00 8.11	Α
	MOTA	710	OG1		109	15.274	1.321	97.857	1.00 5.32	A
	MOTA	711	CG2		109	13.269	0.220	97.079	1.00 2.18	A
70										
, 0	MOTA	712		THR	109	13.914		100.405	1.00 8.77	A
	MOTA	713		THR	109	14.029		101.236	1.00 9.56	A
	MOTA	714		GLY	110	14.411		100.599	1.00 6.93	A
	MOTA	715	CA	GLY	110	15.037	3.517	101.878	1.00 7.00	A
								_		

	MOTA	716		GLY	110	16.491		101.985	1.00 8.39 1.00 6.64	A A
	MOTA	717		GLY	110	17.052		103.089	1.00 8.77	A
	MOTA	718 719		LYS LYS	111 111	17.106 18.493		100.888	1.00 8.41	A
5	MOTA MOTA	720		LYS	111	18.938	5.257	99.495	1.00 9.46	A
3	MOTA	721		LYS	111	19.086	4.134	98.462	1.00 8.41	A
	MOTA	722		LYS	111	19.650	4.651	97.133	1.00 7.10	A
	ATOM	723	CE	LYS	111	18.772	5.741	96.526	1.00 8.55	A
	MOTA	724	NZ	LYS	111	17.364	5.298	96.325	1.00 7.14	A
10	MOTA	725	С	LYS	111	18.643		101.862	1.00 8.34	A
	MOTA	726		LYS	111	19.448		102.789	1.00 9.08	A
	MOTA	727	N	THR	112	17.851		101.651	1.00 8.83 1.00 7.73	A A
	ATOM	728		THR	112	17.896		102.502	1.00 7.73 1.00 8.07	A
15	MOTA	729	CB OG1	THR	112 112	17.027 17.347		101.903	1.00 8.01	Ä
13	MOTA	730 731		THR	112	17.287		102.650	1.00 4.02	A
	MOTA MOTA	732	C	THR	112	17.454		103.945	1.00 8.81	A
	MOTA	733	ŏ	THR	112	17.997		104.894	1.00 8.08	A
	MOTA	734	N	PHE	113	16.476		104.114	1.00 11.03	A
20	MOTA	735	CA	PHE	113	16.008	6.664	105.448	1.00 11.19	A
	MOTA	736	CB	PHE	113	14.806	5.727	105.361	1.00 10.34	A
	MOTA	737	CG	PHE	113	14.208		106.699	1.00 10.76	Α.
	MOTA	738	CD1		113	13.247	6.214	107.276	1.00 9.64	A
25	MOTA	739	CD2		113	14.623		107.393	1.00 9.33	A.
25	MOTA	740	CE1		113	12.703 14.084		108.523	1.00 10.99	A
	MOTA	741 742	CE2	PHE	113 113	13.120		109.212	1.00 9.40	A
	MOTA MOTA	743	c	PHE	113	17.120		106.205	1.00 11.21	A
	MOTA	744	ō	PHE	113	17.254		107.418	1.00 11.83	Α
30	ATOM	745	N	THR	114	17.908	5.159	105.483	1.00 10.89	A
	MOTA	746	CA	THR	114	18.992		106.101	1.00 9.91	A
	MOTA	747	CB	THR	114	19.458		105.173	1.00 12.09	A
	MOTA	748	OG1		114	18.375		105.001	1.00 10.83	A
25:	MOTA	749	CG2		114	20.677		105.763	1.00 9.73	A
35	MOTA	750	C	THR	114	20.167		106.438	1.00 10.11	A A
-	MOTA	751	0	THR	114	20.650		107.569 105.466	1.00 10.30	λ
	MOTA	752 753	N CA	MET	115 115	21.745		105.666	1.00 11.76	A
	MOTA MOTA	754	CB	MET	115	22.286		104.323	1.00 14.08	A
40	ATOM	755	œ	MET	115	22.774		103.406	1.00 21.28	A
. •	ATOM	756	SD	MET	115	24.093		104.142	1.00 28.02	A
	MOTA.	757	CE	MET	115	25.184	6.682	104.670	1.00 16.59	A
	MOTA	758	C	MET	115	21.489		106.547	1.00 11.39	A
4.5	MOTA	759	0	MET	115	22.347		107.349	1.00 11.70	A
45	MOTA	760	N	GLU	116	20.322		106.410	1.00 10.32	Α
	MOTA	761	CA	GLU	116	20.023		107.197	1.00 9.04	A A
	MOTA	762	CB	GLU	116	19.498 20.215		106.299 104.970	1.00 11.83	A
	MOTA	763 764	CG CD	GLU	116 116	19.911		104.319	1.00 17.70	λ.
50	MOTA MOTA	765		GLU	116	18.751		104.405	1.00 20.63	A
50	MOTA	766		GLU	116	20.830		103.715	1.00 19.36	A
	MOTA	767	c	GLU	116	19.021		108.319	1.00 8.57	Α
	ATOM	768	Ó	GLU	116	19.225	10.344	109.430	1.00 6.66	λ
	ATOM	769	N	GLY	117	17.937		108.024	1.00 10.69	A
55	MOTA	770	CA	GLY	117	16.894		109.011	1.00 12.05	A
	MOTA	771	C	GLY	117	15.906		108.921	1.00 14.49	A
	ATOM	772	0	GLY	117	16.009		108.030	1.00 15.09	A
	MOTA	773	N	GLU	118	14.954		109.844	1.00 15.27	A
60	MOTA	774	CA	GLU	118	13.955		109.827	1.00 17.05	Ä
UU	ATOM	775 776	CB	GLU GLU	118 118	12.680 12.881		107.732	1.00 24.85	λ
	MOTA MOTA	777	CG CD	GLU	118	11.659		107.228	1.00 28.50	A
	MOTA	778		GLU	118	11.639		106.047	1.00 29.02	A
	MOTA	779		GLU	118	10.715		108.025	1.00 31.54	A
65	MOTA	780	c	GLU	118	13.601		111.246	1.00 15.85	A
	ATOM	781	ō	GLU	118	14.159	11.111	112.206	1.00 17.29	A
	ATOM	782	N	ARG	119	12.660		111.381	1.00 14.03	A
	MOTA	783	CA	ARG	119	12.238		112.701	1.00 12.36	λ
70	ATOM	784	CB	ARG	119	12.058		112.765	1.00 9.51	A
70	ATOM	785	CG	ARG	119	13.311		112.459	1.00 9.85	A
	MOTA	786	CD	ARG	119	14.517		113.223	1.00 9.11 1.00 11.37	A A
	MOTA	787	NE	ARG	119	14.226		114.632 115.601	1.00 11.37	A
	MOTA	788	CZ	ARG	119	14.274	15.409	113.001	1.00 9.03	~

	atom	789		ARG	119	14.607	16.663 115.326	1.00 8.80	λ
	MOTA	790	NH2	ARG	119	14.003	15.052 116.851	1.00 8.38	A
	ATOM	791	С	ARG	119	10.909	12.278 113.012	1.00 13.30	A
	MOTA	792	0	ARG	119	10.055	12.134 112.140	1.00 12.33	A
5	ATOM	793	N	SER	120	10.746	11.819 114.244	1.00 14.08	A
_		794	CA	SER	120	9.478	11.232 114.630	1.00 14.63	A
	MOTA								
	MOTA	795	CB	SER	120	9.563	10.651 116.037	1.00 13.18	λ
	ATOM	796	OG	SER	120	10.380	9.500 116.043	1.00 13.75	A
	MOTA	797	С	SER	120	8.542	12.434 114.610	1.00 14.70	A
10	ATOM	798	0	SER	120	8.966	13.556 114.877	1.00 14.22	A
- •	ATOM	799	N	PRO	121	7.263	12.222 114.295	1.00 15.80	A
								1.00 15.88	Ä
	MOTA	800	CD	PRO	121	6.629	10.969 113.860		
	MOTA	801	CA	PRO	121	6.312	13.340 114.253	1.00 16.98	A
	MOTA	802	CB	PRO	121	5.037	12.699 113.703	1.00 17.58	A
15	ATOM	803	CG	PRO	121	5.528	11.476 112.967	1.00 18.94	A
	MOTA	804	С	PRO	121	6.036	14.035 115.589	1.00 17.31	A
	ATOM	805	ō	PRO	121	6.316	13.495 116.662	1.00 17.01	A
						5.493	15.249 115.498	1.00 18.27	λ
	ATOM	808	N	ASN	122				
20	ATOM	807	CA	ASN	122	5.079	16.029 116.659	1.00 19.75	A
20	ATOM	808	CB	asn	122	3.899	15.303 117.323	1.00 22.14	A
	ATOM	809	CG	ASN	122	2.806	16.243 117.782	1.00 25.67	A
	ATOM -	810	OD1	ASN	122	2.331	17.090 117.020	1.00 28.24	A
	ATOM	811		ASN	122	2.386	16.089 119.029	1.00 29.36	A
			c	ASN	122	6.137	16.341 117.714	1.00 20.30	A
25	MOTA	812						1.00 19.52	Ä
23	MOTA	813	0	ASN	122	5.810	16.490 118.889		
	MOTA	814	N	GLU	123	7.398	16.443 117.312	1.00 20.21	λ
	MOTA	815	CA	GLU	123	8.460	16.745 118.267	1.00 21.19	A
	MOTA	816	CB	GLU	123	8.341	18.185 118.781	1.00 20.11	A
	MOTA	817	CG	GLU	123	8.519	19.249 117.731	1.00 20.41	A
30	ATOM	818	CD	GLU	123	8.575	20.654 118.319	1.00 21.92	A
	MOTA	819		GLU	123	7.688	21.013 119.133	1.00 18.15	λ
						9.507			Ä
	MOTA	820		GLU	123		21.404 117.951	1.00 21.94	
	MOTA	821	С	GLU	123	B.446	15.806 119.468	1.00 21.37	Α
~~	MOTA	822	0	GLU	123	8.632	16.247 120.602	1.00 19.07	A
35	ATOM	823	N	GLU	124	8.226	14.518 119.233	1.00 22.79	A
	MOTA	824	CA	GLU	124	8.210	13.577 120.339	1.00 22.88	A
	ATOM	825	СВ	GLU	124	7.685	12.215 119.887	1.00 25.26	A
		826	CG	GLÜ	124	7.600	11.205 121.033	1.00 30.44	A
	ATOM								
40	MOTA	827	CD	GLU	124	6.924	9.899 120.636	1.00 34.84	A
40	MOTA	828		GLU	124	6.827	9.003 121.508	1.00 33.81	A
	MOTA	829	OE2	GLU	124	6.494	9.772 119.464	1.00 37.51	A
	ATOM	830	C	GLU	124	9.592	13.404 120.964	1.00 22.45	A
	MOTA	831	0	GLU	124	9.715	13.235 122.180	1.00 23.30	A
	ATOM	832	N	TYR	125	10.635	13.452 120.142	1.00 20.18	A
45	MOTA	833	CA	TYR	125	11.988	13.269 120.657	1.00 19.15	A
		834	CB	TYR	125	12.602	11.953 120.150	1.00 17.84	Ä
	MOTA								
	MOTA	835	CG	TYR	125	11.805	10.695 120.391	1.00 17.89	A
	MOTA	836		TYR	125	10.791	10.304 119.513	1.00 18.58	A
	MOTA	837	CE1	TYR	125	10.086	9.120 119.713	1.00 18.72	A
50	MOTA	838	CD2	TYR	125	12.090	9.871 121.477	1.00 17.89	A
	MOTA	839	CE2	TYR	125	11.395	8.691 121.686	1.00 17.82	A
	MOTA	840	cz	TYR	125	10.398	8.321 120.804	1.00 19.43	A
	MOTA	841	OH	TYR	125	9.724	7.142 121.017	1.00 23.55	A
						12.941	14.377 120.260		A
55	MOTA	842	С	TYR	125				
22	ATOM	843	0	TYR	125	12.678	15.144 119.338	1.00 20.06	A
	MOTA	844	N	THR	126	14.061	14.445 120.971	1.00 18.30	A
	MOTA	845	CA	THR	126	15.106	15.402 120.651	1.00 18.04	A
	MOTA	846	CB	THR	126	16.063	15.618 121.839	1.00 18.63	A
	MOTA	847		THR	126	16.592	14.356 122.254	1.00 20.05	A
60		848		THR	126	15.339	16.258 123.014	1.00 18.83	A
00	MOTA								
	MOTA		C	THR	126		14.653 119.537		A
	MOTA	850	0	THR	126	15.606	13.455 119.355	1.00 16.79	À
	MOTA	851	N	TRP	127	16.708	15.322 118.789	1.00 16.50	A
	MOTA	852	CA	TRP	127	17.401	14.636 117.711	1.00 16.42	Α
65	ATOM	853	CB	TRP	127	18.198	15.642 116.868		A
	MOTA	854		TRP	127	19.443	16.133 117.506		À
			CG					1.00 12.21	
	MOTA	855		TRP	127	20.746	15.554 117.381		A
	MOTA	856		TRP	127	21.634	16.350 118.138		A
	MOTA	857	CE3	TRP	127	21.250	14.436 116.703		A
70	MOTA	858	CD1	TRP	127	19.580	17.225 118.314	1.00 12.48	A
	MOTA	859		TRP	127	20.899	17.365 118.698		A
	MOTA	860		TRP	127	22.997	16.063 118.233		A
				TRP	127	22.607	14.148 116.800		A
	ATOM	861	دع	INF	121	22.007	14.140 110.000	1.00 0.00	· ·

	MOTA	862	CH2	TRP	127	23.463	14.959	117.558	1.00 10.75	A
	MOTA	863	С	TRP	127	18.318		118.191	1.00 18.04	A
	MOTA	864	0	TRP	127	18.496	12.507	117.491	1.00 17.73	Α
	ATOM	865	N	GLU	128	18.874	13.639	119.390	1.00 20.55	Α
5										
,	MOTA	866		GLU	128	19.773		119.954	1.00 22.98	A
	MOTA	867	CB	GLU	128	20.449	13.167	121.216	1.00 24.66	Α
	MOTA	868		GLU	128	21.328		121.028	1.00 30.86	A
	ATOM	869	CD	GLU	128	21.812	14.929	122.359	1.00 34.39	A
	MOTA	870	OE1	CUI	128	22.271	14 126	123.204	1.00 36.58	A
10										
10	ATOM	871	OE2	GLU	128	21.734	16.160	122.562	1.00 36.22	A
	MOTA	872	C	GLU	128	19.092	11.322	120.336	1.00 21.59	A
	ATOM	873	0	GLU	128	19.744	10.291	120.456	1.00 20.67	A
	ATOM	874	N	GLU	129	17.784	11.362	120.539	1.00 22.17	A
	MOTA	875		GLU	129	17.073		120.974	1.00 22.68	A
15										
15	MOTA	876	CB	GLU	129	16.487	10.426	122.364	1.00 23.27	A
	ATOM	877	CG	GLU	129	17.550	10 770	123.392	1.00 28.13	Α
	MOTA	878	CD	GLU	129	16.965	11.15/	124.737	1.00 32.95	A
	MOTA	879	OE1	GLU	129	17.752	11.323	125.702	1.00 33.26	A
	ATOM	880	OE2		129	15.724		124.827	1.00 31.63	A
20										
20	MOTA	881	С	GLU	129	. 15.983	9.679	120.035	1.00 20.72	A
	ATOM	882	0	GLU	129	15.273	8.728	120.343	1.00 23.09	A
	MOTA	883		ASP	130	15.862		118.885	1.00 18.40	Α.
	ATOM	884	CA	ASP	130	14.846	9.945	117.918	1.00 16.36	A
	ATOM	.885		ASP	130	14.770		116.828	1.00 15.71	A
25										
25	MOTA	886	CG	ASP	130	13.495	10.947	116.031	1.00 15.49	A
	MOTA	887	OD1	ASP	130	13.044	12 002	115.545	1.00 17.27	A
	MOTA	888	OD2	ASP	130	12.950	9.839	115.874	1.00 15.06	A
	MOTA	889	C .	ASP	130	15:168	8.573	117.326	1.00 15.41	A
	ATOM	890			130	16.196			1.00 15.65	A
20				ASP				116.680		
30	ATOM	891	N	PRO	131	14.287	7.597	117.548	1.00 14.81	A
	ATOM	892	CD	PRO	131	12.980	7 675	118.222	1.00 14.52	A
	ATOM	893	CA	PRO	131	14.523	6.255	117.018	1.00 15.02	A
	ATOM	894	CB	PRO	131	13.348	5.457	117.579	1.00 15.21	A
25.	ATOM	895		PRO	131	12.267		117.656	1.00 16.02	A
35	ATOM	- 896	С	PRO	131	14.607	6.183	115.492	1.00 15.04	A
	ATOM	897	0	PRO	131	15.103	5 196	114.943	1.00 12.71	A
	MOTA	898	N	LEU	132	14.125	1.224	114.814	1.00 14.88	A
	MOTA	899	CA	LEU	132	14.161	7.254	113.354	1.00 14.03	A
40	MOTA	900		LEU	132	12.947		112.796	1.00 12.82	A
40	MOTA	901	CG	LEU	132	11.562	7.434	113.129	1.00 14.44	A
	ATOM	902	CD1	LEH	132	10.506	8 271	112.397	1.00 8.97	A
	ATOM	903	CD2	LEU	132	11.470	5.950	112.724	1.00 8.90	A
	ATOM	904	С	LEU	132	. 15.446	7., 861	112.786	1.00 12.21	A
	ATOM	905		LEU	132			111.573	1.00 11.16	λ
15						15.626				
45	MOTA	906	N.	ALA	133	16.337	8.321	113.655	1.00 11.83	A
	ATOM	907	CA .	ALA	133	17.604	8 891	113.186	1.00 11.94	A
	MOTA	908	CB .	ALA	133	18.447	9.345	114.377	1.00 7.70	A
	ATOM	909	С.	ALA	133	18.367	7.825	112.373	1.00 12.53	Α
	ATOM	910		ALA	133	18.308		112.693	1.00 12.95	A
50										
50	MOTA	911	N I	GLY	134	19.074	8.256	111.330	1.00 13.23	A
	MOTA	912	CA	GLY	134	19.832	7.328	110.506	1.00 13.31	A
	MOTA	913	C	GLY	134	21.314		110.858	1.00 14.51	A
	MOTA	914	0	GLY	134	21.727	7.771	111.910	1.00 12.96	A
	MOTA	915	N	ILE	135	22.111	6 685	109.962	1.00 13.27	A
55										
"	ATOM	916	CX	ILE	135	23.547	6.529	110.158	1.00 10.64	A
	ATOM	917	CB	ILE	135	24.211	5.825	108.945	1.00 12.21	Α
	MOTA	918	CG2		135	25.728		109.166	1.00 9.26	A
	ATOM	919	CG1	ILE	135	23.606	4.433	108.749	1.00 9.44	A
	MOTA	920	CD1	TLE	135	24.194	3 659	107.563	1.00 7.34	A
60										
60	ATOM	921	С	ILE	135	24.319		110.429	1.00 11.04	A
	ATOM	922	0	ILE	135	25.101	7.868	111.370	1.00 12.98	A
							0.043			
	ATOM	923		ILE	136	24.117		109.606	1.00 10.10	A
	MOTA	924	CA	ILE	136	24.822	10.109	109.783	1.00 10.16	A
	ATOM	925		ILE	136	24.393		108.709	1.00 9.76	A
65										
65	MOTA	926	CG2	ILE	136	25.052	12.489	108.966	1.00 7.05	A
	ATOM	927	CG1		136	24.783		107.327	1.00 8.04	A
	MOTA	928	CD1		136	24.420		106.177	1.00 8.70	A
	ATOM	929	C	ILE	136	24.680	10.734	111.180	1.00 10.98	A
		930								
70	MOTA			ILE	136	25.673		111.848	1.00 11.07	λ
70	MOTA	931	N :	PRO	137	23.449	11.015	111.637	1.00 12.76	A
	MOTA	932		PRO	137	22.118		111.018	1.00 12.91	A
	MOTA	933	CA .	PRO	137	23.344	11.609	112.974	1.00 13.27	A
	MOTA	934	CB :	PRO -	137	21.863	11.966	113.079	1.00 12.28	A
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		036								_
	MOTA	935	CG	PRO	137	21.210		112.226	1.00 12.44	A
	ATOM	936	С	PRO	137	23.814		114.117	1.00 13.75	A
	MOTA	937	0	PRO	137	24.349		115.118	1.00 13.93	A
5	MOTA	938	N	ARG	138	23.616		113.982	1.00 13.99	A
ے	MOTA	939	CA	ARG	138	24.061		115.034	1.00 14.63	A
	MOTA	940	CB	ARG	138	23.520		114.788	1.00 11.07	A
	ATOM	941	CC	ARG	138	22.026		115.030	1.00 10.07	A
	MOTA	942	CD	ARG	138	21.514		114.706	1.00 12.89	A
10	MOTA	943	NE	ARG	138	20.063	5.502	114.816	1.00 14.12	A
10	MOTA	944	CZ	ARG	138	19.395	5.417	115.961	1.00 16.84	A
	MOTA	945	NH1	ARG	138	20.043	5.380	117.123	1.00 17.01	A
	ATOM	946	NH2	ARG	13B	18.070	5.405	115.943	1.00 16.58	A
	ATOH	947	С	ARG	138	25.590	8.479	115.105	1.00 14.82	Α
	MOTA	948	0	ARG	138	26.175	8.491	116.189	1.00 17.18	A
15	MOTA	949	N	THR	139	26.227	8.490	113.943	1.00 13.19	A
	ATOM	950	CA	THR	139	27.676	8.487	113.864	1.00 14.27	A
	MOTA	951	CB	THR	139	28.134	8.347	112.394	1.00 15.10	· A
	ATOH	952	OG1	THR	139	27.671	7.092	111.877	1.00 16.74	A
	MOTA	953	CG2	THR	139	29.663	8.403	112.290	1.00 15.25	A
20	ATOM	954	С	THR	139	28.315	9.738	114.473	1.00 14.96	A
	MOTA	955	0	THR	139	29.268	9.642	115.247	1.00 16.32	A
	MOTA	956	N	LEU	140	27.802	10.912	114.128	1.00 13.16	A
	MOTA	957	CA	LEU	140	28.374	12.136	114.664	1.00 13.55	A
	MOTA	958	СВ	LEU	140	27.742		113.988	1.00 13.68	A
25	ATOM	959	CC	LEU	140	28.065		112.489	1.00 15.01	A
	MOTA	960	CD1	LEU	140	27.116		111.824	1.00 15.28	A
	MOTA	961		LEU	140	29.535		112.286	1.00 12.18	A
	ATOM	962	C	LEU	140	28.168		116.165	1.00 14.55	A
	ATOM	963	0	LEU	140	29.031		116.900	1.00 14.87	A
30	MOTA	964	N	HIS	141	27.021		116.621	1.00 15.53	A
-	MOTA	965	CA	HIS	141	26.715		118.041	1.00 15.51	A
	ATOM	966	СВ	HIS	141	25.241		118.265	1.00 17.50	A
	ATOM	967	CG	HIS	141	24.809		119.698	1.00 19.49	A
	MOTA	968		HIS	141	24.144		120.400	1.00 20.09	A
35	ATOM	969		HIS	141	25.057		120.584	1.00 22.94	A
	ATOM	970		HIS	141	24.561		121.769	1.00 21.94	A
	ATOM	971		HIS	141	24.002		121.683	1.00 21.59	Α
	MOTA	972	C	HIS	141	27.638		118.787	1.00 14.45	A
	MOTA	973	ŏ	HIS	141	28.133		119.864	1.00 12.82	A
40	MOTA	974	N	GLN	142	27.893		118.202	1.00 12.87	A
	MOTA	975	CA	GLN	142	28.753		118.852	1.00 14.02	Ä
	MOTA	976	CB	GLN	142	28.542		118.239	1.00 13.39	A
	MOTA	977	CC	GLN	142	27.299		118.741	1.00 20.05	Ä
	ATOM	978	CD	GLN	142	27.237		120.262	1.00 21.32	A
45	ATOM	979		GLN	142	26.660		120.910	1.00 21.37	Ä
	MOTA	980		GLN	142	27.850		120.837	1.00 19.74	Ä
	MOTA	981	c	GLN	142	30.243		118.862	1.00 13.74	A
	MOTA	982	ŏ	GLN	142	30.961		119.759	1.00 14.17	Ä
	MOTA	983	N	ILE	143	30.713		117.870	1.00 13.21	Ä
50	ATOM	984	CA	ILE	143	32.119		117.826	1.00 13.39	A
	ATOM	985	CB	ILE	143	32.435		116.576	1.00 11.43	A
	MOTA	986		ILE	143	33.847		116.678	1.00 13.15	A
	ATOM	987		ILE	143	32.282		115.324	1.00 9.90	A
	ATOM	988		ILE	143	32.437		114.012	1.00 8.46	A
55	ATOM	989	c	ILE	143	32.454		119.082	1.00 14.99	Ä
	ATOM	990	ŏ	ILE	143	33.473		119.724	1.00 13.04	A
	ATOM	991	N	PHE	144	31.581		119.419	1.00 17.68	Ä
	ATOM	992	CA	PHE	144	31.741		120.599	1.00 20.78	Ä
	ATOM	993	СВ	PHE	144	30.771		120.548	1.00 17.56	Ä
60	ATOM	994	CG	PHE	144	31.153		119.549	1.00 18.09	A
00	MOTA	995		PHE	144	32.205		119.809		
									1.00 18.10	A
	ATOM	995 997		PHE	144 144	30.492 32.596		118.327	1.00 17.52	A
	ATOM			PHE		32.596		118.864	1.00 19.03	A
65	MOTA	998			144			117.371	1.00 16.50	A
05	ATOM	999	CZ	PHE	144	31.926		117.639	1.00 18.32	A
	ATOM	1000	C	PHE	144	31.481		121.877	1.00 24.06	A
	MOTA	1001	0	PHE	144	32.059		122.917	1.00 25.61	A
	MOTA	1002	N	GLU	145	30.596		121.801	1.00 28.05	A
70	MOTA	1003	CA	GLU	145	30.270		122.963	1.00 32.18	A
70	ATOM	1004	CB	GLU	145	29.052		122.660	1.00 34.92	A
	MOTA	1005	CG	GLU	145	28.382		123.877	1.00 41.48	A
	MOTA	1006	CD	GLU	145	27.459		124.604	1.00 46.68	Α
	ATOM	1007	UEI	GLU	145	26.808	9.154	125.583	1.00 48.85	A

	MOTA	1008	UE3	GLU	145	27.379	10.772 1	24 205	1.00 48.27	A
		1000			145		9.234		1.00 33.53	Ä
	MOTA		c	GLU		31.472			1.00 35.14	Ä
	MOTA	1010	0	GLU	145 146	31.796	9.031 1		1.00 33.94	Ä
5	MOTA	1011	N	LYS		32.139	8.727 1 7.857 1		1.00 35.62	Ä
J	ATOM	1012	CA	LYS	146 146	33.289	6.982 1		1.00 35.76	Ä
	ATOM	1013	CB	LYS		33.493			1.00 38.40	Â
	ATOM	1014	CG	LYS	146	32.398	5.949 1		1.00 39.00	
	MOTA	1015	CD	LYS	146	32.750	5.000 1			A
10	ATOM	1016	CE	LYS	146	31.822	3.804 1		1.00 40.55	A
10	MOTA	1017	NZ	LYS	146	32.108	2.871 1		1.00 42.99	A
	MOTA	1018	C	LYS	146	34.600	8.572 1		1.00 37.30	A
	ATOM	1019	0	LYS	146	35.279	8.224 1		1.00 38.30	λ
	MOTA	1020	N	LEU	147	34.959	9.567		1.00 37.75	A
15	MOTA	1021	CA	LEU	147	36.212	10.286 1		1.00 39.45	A
15	MOTA	1022	CB	LEU	147	36.611	11.013 1		1.00 36.70	λ
	MOTA	1023	CG	LEU	147	36.769	10.134		1.00 34.99	A
	ATOM	1024		LEU	147	37.244	10.979		1.00 32.76	A
	ATOM	1025		LEU	147	37.754	9.012		1.00 33.24	À
20	MOTA	1026	C	LEU	147	36.250	11.268		1.00 41.40	A
20	MOTA	1027	0	LEU	147	37.329	11.653		1.00 41.57	A
	MOTA	1028	N	THR	148	35.091	11.681		1.00 43.50	A
	HOTA	1029	CA	THR	148	35.078	12.613		1.00 46.76	λ.
	ATOM	1030	CB	THR	148	33.735	13.379		1.00 46.73	A
25	MOTA	1031		THR	148	33.559	14.194		1.00 45.09	. A
25	ATOM	1032		THR	148	33.717	14.274		1.00 45.59	A
	MOTA	1033	С	THR	148	35.327	11.848		1.00 50.09	Ä
	MOTA	1034	0	THR	148	36.050	12.321 1		1.00 50.49	A
	MOTA	1035	N	ASP	149	34.734	10.660		1.00 53.41	A
20	ATOM	1036	CA	ASP	149	34.899		127.545	1.00 56.45	A
30	ATOM	1037	CB	ASP	149	34.094		127.395	1.00 57.31	A
	MOTA	1038	CG	ASP	149	32.677		127.926	1.00 59.22	A
	ATOM	1039		ASP	149	32.519		129.090	1.00 59.37	A
	ATOM	1040		ASP	149	31.723	8.302		1.00 59.44	A
35	ATOM	1041	C	ASP	149	36.365		127.778	1.00 57.60	A
33	MOTA	1042	0	ASP	149	36.948		128.800	1.00 57.84	A
	ATOM	1043	N	ASN	150	36.955		126.824	1.00 58.66	A
	ATOM	1044	CA	ASN	150	38.354		126.919	1.00 59.63	A
	ATOM	1045	CB	ASN	150	38.699		125.793	1.00 62.63	A A
40	MOTA	1046	CC	ASN	150	37.845		125.832	1.00 65.36	
40	ATOM	1047		ASN	150	37.880		126.803	1.00 66.45	A A
	MOTA	1048		ASN	150	37.070		124.774	1.00 58.25	Ā
	ATOM	1049	c	ASN	150	39.248	10.657	126.833	1.00 58.50	Ä
	ATOM	1050	0	ASN GLY	150 151	38.814 40.492		127.279	1.00 56.63	Ã
45	ATOM	1051	N				10.579		1.00 55.03	Â
7.7	MOTA	1052	CA C	GLY GLY	151 151	41.416 41.915	10.801		1.00 53.26	Ä
	MOTA	1053 1054		GLY	151	42.983	10.307		1.00 52.83	A
	MOTA MOTA	1055	O N	THR	152	41.149	11.551		1.00 50.83	A
	ATOM	1056	CA	THR	152	41.519	11.806		1.00 47.73	Ä
50	ATOM	1057	CB	THR	152	40.763	10.858		1.00 47.39	Ä
50	ATOM	1058		THR	152	40.890		123.127	1.00 48.20	A
	ATOM	1059		THR	152	41.326	10.975		1.00 45.61	λ
	HOTA	1060	C	THR	152	41.237	13.230		1.00 46.24	A
	MOTA	1061	ŏ	THR	152	40.163	13.775		1.00 46.24	Ä
55	ATOM	1062	N	GLU	153	42.217	13.828		1.00 43.69	A
33	MOTA	1063	CA	GLU	153	42.066	15.165		1.00 41.25	A
	ATOM	1064	CB	GLU	153	43.386	15.926		1.00 42.93	A
	MOTA	1065	CG	GLU	153	43.815	16.330		1.00 46.50	Ä
	MOTA	1066	CD	GLU	153	45.193	16.952		1.00 48.91	A
60 ·	ATOM	1067		GLU	153	46.181	16.219		1.00 49.46	A
00	MOTA	1068		GLU	153		18.177		1.00 52.22	A
	MOTA	1069	C	GLU	153	41.677	14.898		1.00 38.96	A
	MOTA	1070	ò	GLU	153	42.232	13.998		1.00 38.36	Ä
	ATOM	1071	N	PHE	154	40.730	15.665		1.00 35.01	Ä
65	MOTA	1071	CA	PHE	154	40.289	15.434		1.00 30.73	Ä
J J	MOTA	1072	CB	PHE	154	39.416	14.177		1.00 27.60	Ä
	ATOM	1074	CG	PHE	154	38.102	14.340		1.00 24.32	Â
	ATOM	1075		PHE	154	36.965	14.742		1.00 22.22	Ä
	MOTA	1076		PHE	154	38.009	14.130		1.00 24.15	A
70	ATOM	1075		PHE	154	35.751	14.130		1.00 22.43	Ä
, 0	ATOM	1077		PHE	154	36.797	14.325		1.00 24.33	Ä
	ATOM	1078	CZ	PHE	154	35.664	14.718		1.00 23.63	À
	ATOM	1080	C	PHÉ	154	39.498	16.590		1.00 28.48	Ä
	WI OH	1000	•	FIL	134	37.430	10.330	-10.024	2.00 20.40	**

	MOTA	1081	0	PHE	154	38.921	17.402	118.744	1.00 27.87	A
	MOTA	1082	N	SER	155	39.474	16 653	116.702	1.00 26.86	Α
	MOTA	1083	CA	SER	155	38.713	_	116.006	1.00 25.68	A
_	MOTA	1084	CB	SER	155	39.635	18.708	115.347	1.00 24.22	A
5	MOTA	1085	OG	SER	155	40.401	18.131	114.309	1.00 25.09	A
	ATOM	1086	Ċ	SER	155	37.920		114.947	1.00 26.10	A
						38.402				
	ATOM	1087	0	SER	155			114.380	1.00 26.26	A
	MOTA	1088	N	VAL	156	36.697	17.377	114.700	1.00 25.35	A
	MOTA	1089	CA	VAL	156	35.836	16.741	113.712	1.00 23.66	A
10	ATOM	1090	CB	VAL	156	34.549		114.371	1.00 22.75	A
	ATOM	1091		VAL	156	33.671		113.331	1.00 20.72	A
	MOTA	1092	CG2	VAL	156	34.910	15.257	115.497	1.00 20.01	A
	MOTA	1093	С	VAL	156	35.447	17.733	112.622	1.00 24.01	A
	ATOM	1094	0	VAL	156	34.960	18.832	112.916	1.00 24.09	A
15	ATOM	1095	N	LYS	157	35.679		111.369	1.00 21.25	A
13										
	MOTA	1096	CA	LYS	157	35.332		110.220	1.00 20.34	, А
	MOTA	1097	CB	LYS	157	36.559	18.467	109.347	1.00 24.12	A
	MOTA	1098	CG	LYS	157	37.755	19.140	110.028	1.00 28.05	A
	MOTA	1099	CD	LYS	157	37.474		110.410	1.00 31.98	A
20										
20	MOTA	1100	CE	LYS	157	38.755		110.845	1.00 35.17	A
	MOTA	1101	NZ	LYS	157	39.737	21.545	109.726	1.00 35.98	A
	ATOM	1102	С	LYS	157	34.333	17.380	109.382	1.00 19.05	A
	MOTA	1103	0	LYS	157	34.475	16.166	109.209	1.00 18.10	A
	ATOM	1104	N	VAL	158	33.315		108.865	1.00 15.97	A
25										
23	MOTA	1105	CA	VAL	158	32.340		108.025	1.00 14.22	A
	MOTA	1106	CB	VAL	158	30.941	17.281	108.690	1.00 12.88	A
	MOTA	1107	CG1	·VAL	158	31.014	16.411	109.931	1.00 10.13	A
	ATOM	1108		VAL	158	30.419	18 651	109.031	1.00 13.23	A
								106.706	1.00 13.72	
20	MOTA	1109	C	VAL	158	32.221				A
30	MOTA	1110	0	VAL	158	32.469	19.300	106.610	1.00 14.66	A
	MOTA	1111	N	SER	159	31.845	17.373	105.677	1.00 14.86	A
	ATOM	1112	CA	SER	159	31.702	17.955	104.362	1.00 16.10	. А
	ATOM	1113	CB	SER	159	33.034		103.618	1.00 17.14	Α
25	ATOM	1114	OG	SER	159	32.904		102.279	1.00 23.83	A
35	MOTA	1115	С	SER	159	30.609		103.642	1.00 15.89	A
	MOTA	1116	0	SER	159	30.477	15.976	103.B22	1.00 15.28	A
	MOTA	1117	N	LEU	160	29.820		102.838	1.00 15.69	A
						2B.728		102.098	1.00 15.26	A
	MOTA	1118	CA	LEU	160					
40	MOTA	1119	CB	LEU	160	27.388		102.715	1.00 15.28	A
40	MOTA	1120	CG	LEU	160	26.121	17.071	102.104	1.00 15.37	A
	MOTA	1121	CD1	LEU	160	26.236	15.559	102.087	1.00 12.97	A
	ATOM	1122		LEU	160	24.904		102.904	1.00 14.38	A
	ATOM	1123	C	LEU	160	28.799		100.640	1.00 15.74	A
4	MOTA	1124	0	LEU	160	28.331	18.766	100.263	1.00 15.17	A
45	MOTA	1125	N	LEU	161	29.394	16.822	99.829	1.00 15.44	A
	MOTA	1126	CA	LEU	161	29.577	17.052	98.401	1.00 15.04	A
	ATOM	1127	CB	LEU	161	30.923	16.472	97.968	1.00 16.39	Α
	MOTA	1128	CG	LEU	161	31.753	17.038	96.815	1.00 19.66	A
~~	MOTA	1129		LEU	161	32.749	15.955	96.386	1.00 20.66	A
50	MOTA	1130	CD2	LEU	161	30.887	17.437	95.641	1.00 20:16	A
	MOTA	1131	С	LEU	161	28.470	16.311	97.680	1.00 15.70	A
	ATOM	1132	ō	LEU	161	28.200	15.161	97.989	1.00 17.10	Α
	ATOM	1133	N	GLU	162	27.829	16.952	96.713	1.00 15.78	A
~ ~	MOTA	1134	CA	GLU	162	26.763	16.286	95.984	1.00 13.96	A
55	ATOM	1135	СВ	GLU	162	25.413	16.834	96.428	1.00 14.46	A
	ATOM	1136	CG	GLU	162	25.218	16.645	97.928	1.00 17.99	A
	MOTA	1137	CD	GLU	162	23.781	16.776	98.372	1.00 18.53	A
	MOTA	1138		GLU	162	23.532	16.663	99.588	1.00 20.86	A
	ATOM	1139	OE2	GLU	162	22.902	16.984	97.513	1.00 17.99	A
60	ATOM	1140	С	GLU	162	26.948	16.403	94.489	1.00 12.56	A
•	ATOM	1141	ō	GLU	162	27.425		93.985	1.00 12.95	A
								93.782	1.00 11.75	
	MOTA	1142	N	ILE	163	26.575	15.346			A
	MOTA	1143	CA	ILE	163	26.736	15.303	92.340	1.00 11.19	A
	MOTA	1144	CB	ILE	163	27.588	14.077	91.941	1.00 10.80	A
65	MOTA	1145		ILE	163	27.790	14.044	90.436	1.00 9.29	A
-	MOTA	1146		ILE	163	28.927	14.121	92.681	1.00 10.31	A
	MOTA	1147		ILE	163	29.667	12.777	92.718	1.00 12.19	A
	MOTA	1148	С	ILE	163	25.393	15.238	91.626	1.00 11.81	A
	ATOM	1149	0	ILE	163	24.524	14.441	91.985	1.00 13.50	A
70	ATOM	1150	N	TYR	164	25.228	16.089	90.620	1.00 10.80	A
				TYR		24.011		89.826	1.00 11.96	Ä
	ATOM	1151	CA		164		16.125			
	MOTA	1152	CB	TYR	164	23.038	17.194	90.353	1.00 11.56	A
	MOTA	1153	CG	TYR	164	21.746	17.240	89.573	1.00 10.77	A

	MOTA	1154	CD1	TYR	164	21.639	18.005	88.408	1.00 9.75	A
	MOTA	1155	CEI		164	20.479	17.991	87.638	1.00 8.60	λ
	MOTA	1156		TYR	164	20.653	16.457	89.954	1.00 8.92	λ
	ATOM	1157	CES		164	19.483	16.428	89.187	1.00 9.51	λ
5	MOTA	1158	cz	TYR	164	19.405	17.197	88.031	1.00 10.37	A
_	MOTA	1159	ОН	TYR	164	18.264	17.167	87.261	1.00 9.00	A
	MOTA	1160	c.	TYR	164	24.415	16.443	88.395	1.00 12.68	Ä
	MOTA	1161	ō	TYR	164	25.048	17.468	88.131	1.00 13.49	λ
	MOTA	1162	N	ASN	165	24.075	15.550	87.478	1.00 12.65	A
10	ATOM	1163	Cλ	ASN	165	24.410	15.745	86.078	1.00 14.45	λ
10	MOTA	1164	CB		165	23.541	16.864	85.515	1.00 18.24	A
	MOTA		CG	asn					1.00 24.46	A
	MOTA	1165 1166			165 165	23.498	16.869	84.010	1.00 29.01	Â
						23.396 23.556	15.817	83.374 83.422	1.00 27.99	Â
15	MOTA	1167		ASN	165		18.061			
13	MOTA	1168	C	ASN	165	25.903	16.069	85.930	1.00 14.74 1.00 13.82	A A
	MOTA	1169	0	ASN	165	26.290	16.972	85.184	1.00 13.82	
	MOTA	1170	N	GLU	166	26.729	15.321	86.663		À
	MOTA	1171	CA	GLU	166	28.178	15.475	86.645	1.00 13.84	A
20	MOTA	1172	CB	GLU	166	28.730	15.118	85.265	1.00 11.37	A
20	MOTA	1173	CC	GLU	166	28.676	13.635	84.952	1.00 13.48	A
	ATOM	1174	CD	GLU	166	29.270	12.781	86.069	1.00 15.85	A
	MOTA	1175		GLU	166	28.518	12.411	86.995	1.00 14.50	Α.
	ATOM	1176		GLU	166	30.491	12.490	86.022	1.00 14.74	A
25	MOTA	1177	C	GLU	166	28.724	16.835	87.067	1.00 15.33	λ
23	MOTA	1178	0	GLU	166	29.809	17.229	86.650	1.00 16.01	A
	MOTA	1179	N	GLU	167	27.970	17.555	87.885	1.00 16.84	λ
	MOTA	1180	CA	GLU	167	28.415	18.850	88.381	1.00 16.72	A
	MOTA	1181	CB	GLU	167	27.403	19.949	88.052	1.00 19.43	A
30	MOTA	1182	CG	GLU	167	27.235	20.216	86.570	1.00 23.50	A
30	ATOM	1183	CD	GLU	167	26.307	21.388	86.309	1.00 28.67	A
	MOTA	1184		GLU	167	25.176	21.382	86.846	1.00 32.20	λ
	MOTA	1185		GLU	167	26.707	22.316	85.571	1.00 31.83	A
	MOTA	1186	C	GLU	167	28.522	18.685	89.888	1.00 15.13	A
25	MOTA	1187	0	GLU	167	27.773	17.908	90.480	1.00 15.63	A
35	ATOM	·1188	N	LEU	168	29.449	19.408	90.501	1.00 12.84	A
	MOTA	1189	CA	LEU	168	29.672	19.312	91.939	1.00 12.94	A
	MOTA	1190	CB	LEU	168	31.171	19.220	92.217	1.00 14.17	A
	MOTA	1191	CG	LEU	168	31.859	17.853	92.232	1.00 18.45	A
40	ATOM	1192		LEU	168	31.289	16.947	91.164	1.00 19.30	A
40	MOTA	1193		LEU	168	33.366	18.058	92.047	1.00 18.21	A
	MOTA	1194	С	LEU	168	29.080	20.467	92.732	1.00 11.51	A
	MOTA	1195	0	LEU	168	29.228	21.631	92.357	1.00 12.03	A
	MOTA	1196	N	PHE	169	28.415	20.138	93.834	1.00 8.76	A
15	MOTA	1197	CA	PHE	169	27.812	21.152	94.682	1.00 10.79	A
45	MOTA	1198	CB	PHE	169	26.286	21.155	94.543	1.00 8.69	A
	MOTA	1199	CG	PHE	169	25.804	21.329	93.127	1.00 9.29	A
	MOTA	1200		PHE	169	25.568	20.219	92.314	1.00 8.53	A
	MOTA	1201		PHE	169	25.605	22.595	92.598	1.00 7.95	A
50	MOTA	1202		PHE	169	25.140	20.372	90.996	1.00 9.35	A
50	ATOM	1203		PHE	169	25.178	22.762	91.284	1.00 7.75	A
	MOTA	1204	CZ	PHE	169	24.945	21.648	90.479	1.00 9.59	A
	MOTA	1205	C	PHE	169	28.187	20.923	96.138	1.00 12.65	λ
	MOTA	1206	0	PHE	169	28.319	19.788.	96.593	1.00 13.12	A
55	ATOM	1207	N	ASP	170	28.369	22.027	96.850	1.00 12.7B	λ
22	MOTA	1208	CA	ASP	170	28.724	22.018	98.253	1.00 13.35	A
	MOTA	1209	CB	ASP	170	29.817	23.060	98.502	1.00 12.29	A
	MOTA	1210	CG	ASP	170	30.300	23.072	99.931	1.00 13.08	A
	MOTA	1211		ASP	170	29.577		100.817	1.00 14.08	A
60	MOTA	1212		ASP	170	31.404		100.176	1.00 15.39	λ
60	MOTA	1213	С	ASP	170	27.456	22.413	99.001	1.00 15.21	A
	MOTA	1214	0	ASP	170		23.588	99.003	1.00 13.76	A
	MOTA	1215	N	LEU	171	26.797	.21.445	99.635	1.00 16.64	A
	MOTA	1216	CA	LEU	171	25.563		100.365	1.00 19.47	A
C 5	MOTA	1217	CB	LEU	171	24.650		100.376	1.00 18.16	A
65	MOTA	1218	CG	LEU	171	23.677	20.315	99.200	1.00 20.70	A
	MOTA	1219	CD1		171	22.739	21.515	99.130	1.00 21.59	A
	ATOM	1220	CD2		171	24.436	20.192	97.900	1.00 19.74	A
	MOTA	1221	С	LEU	171	25.724		101.794	1.00 21.95	A
20	ATOM	1222	0	LEU	171	24.747	22.282	102.536	1.00 24.93	A
70	MOTA	1223	N	LEU	172	26.931	22.618	102.197	1.00 24.33	A
	MOTA	1224	CA	LEU	172	27.108	23.129	103.558	1.00 25.95	A
	MOTA	1225	CB	LEU	172	28.101		104.353	1.00 22.64	A
	MOTA	1226	CG	LEU	172	27.683	20.835	104.713	1.00 21.08	A

	MOTA	1227	CDI	LEU	172	28.747	20.208	105.584	1.00 19.49	A
	ATOM	1228	CD2	LEU	172	26.353		105.450	1.00 20.02	A
	ATOM	1229	C	LEU	172	27.550		103.579	1.00 28.46	A
_	MOTA	1230	0	LEU	172	27.222	25.328	104.512	1.00 33.47	A
5	MOTA	1231	N	ASN	173	28.280	25.020	102.557	1.00 27.52	. У
	MOTA	1232	CA	ASN	173	28.733		102.479	1.00 28.63	A
	ATOM	1233	CB	ASN	173	29.491		101.166	1.00 28.72	Ą
	MOTA	1234	CC	ASN	173	30.022	28.037	101.013	1.00 30.51	A
	MOTA	1235	OD1	ASN	173	30.709	28.350	100.03B	1.00 32.23	A
10	ATOM	1236	ND2		173	29.709		101.969	1.00 31.50	A
	ATOM	1237	С	ASN	173	27.514		102.555	1.00 30.66	A
	MOTA	1238	0	ASN	173	26.639		101.688	1.00 30.81	A
	ATOM	1239	N	PRO	174	27.434	28.164	103.602	1.00 32.10	A
	MOTA	1240	CD	PRO	174	28.196	28 086	104.862	1.00 32.35	A
15	ATOM	1241	CA	PRO	174	26.298		103.741		A
10									1.00 34.00	
	ATOM	1242	CB	PRO	174	26.085		105.243	1.00 33.56	A
	MOTA	1243	CG	PRO	174	27.500	29.119	105.740	1.00 33.25	A
	MOTA	1244	С	PRO	174	26.566	30.469	103.179	1.00 35.77	A
	ATOM	1245	ŏ	PRO	174	26.014		103.667	1.00 38.93	A
20										
20	MOTA	1246	N	SER	175	27.404		102.155	1.00 36.48	A
	MOTA	1247	CA	SER	175	27.734	31.848	101.568	1.00 36.56	A
	MOTA	1248	CB	SER	175	29.104	32.312	102.064	1.00 36.53	A
	ATOM	1249	OG	SER	175	29.142	32.334	103.481	1.00 38.61	λ
	MOTA	1250	Ċ	SER	175		31.745	100.059	1.00 36.99	A
25						27.746				
23	MOTA	1251	0	SER	175	28.234	32.639	99.366	1.00 37.49	· A
	MOTA	1252	N	SER	176	27.226	30.631	99.560	1.00 37.22	. A
	ATOM	1253	CA	SER	176	27.142	30.385	98.125	1.00 38.02	A
	ATOM	1254	CB	SER	176	28.296	29.483	97.662	1.00 37.78	A
	ATOM	1255				28.200	28.177			
30			OG	SER	176			98.213	1.00 37.44	λ
20	MOTA	1256	С	SER	176	25.807	29.699	97.862	1.00 37.53	A
	ATOM	1257	0	SER	176	25.277	29.016	98.734	1.00 37.34	A
	MOTA	1258	N	ASP	177	25.248	29.891	96.676	1.00 38.02	A
	ATOM	1259	CA	ASP	177	23.983	29.243	96.366	1.00 39.18	A
25	MOTA	1260	CB	ASP	177	23.012	30.229	95.704	1.00 41.03	A
35	ATOM	1261	CG	ASP	177	23.585	30.879	94.466	1.00 42.23	A
	MOTA	1262	OD1	ASP	177	23.936	30.156	93.511	1.00 43.11	Α
	MOTA	1263	002	ASP	177	23.679	32.122	94.447	1.00 44.29	A
	MOTA	1264	c	ASP	177			95.471		
						24.219	28.031			λ
40	MOTA	1265	0	ASP	177	25.274	27.910	94.849	1.00 37.31	A,
40	MOTA	1266	N	VAL	178	23.232	27.141	95.415	1.00 38.30	A
	ATOM	1267	CA	VAL	178	23.329	25.918	94.626	1.00 38.53	A
	ATOM	1268	CB	VAL	178	22.091	25.018	94.830	1:00 38.67	λ
	ATOM									
		1269	CG1		178	22.040	24.532	96.266	1.00 38.55	A
45	MOTA	1270	CG2		178	20.828	25.780	94.472	1.00 38.63	A
45	MOTA	1271	С	VAL	178	23.526	26.111	93.129	1.00 38.49	A
	MOTA	1272	0	VAL	178	23.589	25.138	92.385	1.00 39.24	A
	MOTA	1273	N	SER	179	23.618	27.357	92.683	1.00 38.10	A
	MOTA	1274	CA	SER	179	23.823	27.626	91.268	1.00 37.56	A
50	MOTA	1275	CB	SER	179	23.265	29.000	90.905	1.00 39.68	A
50	MOTA	1276	OG	SER	179	21.942	29.155	91.390	1.00 45.54	. А
	MOTA	1277	С	SER	179	25.318	27.594	90.981	1.00 36.56	A
	ATOM	1278	ō	SER	179	25.740	27.516	89.828	1.00 37.57	A
	MOTA	1279	N	GLU	180	26.112	27.663	92.044		A
~~	ATOM	1280	CA	GLU	180	27.566	27.651	91.938	1.00 34.69	A
55	MOTA	1281	CB	GLU	180	28.173	28.564	93.018	1.00 36.86	A
	MOTA	1282	CG	GLU	180	27.906	30.055	92.767	1.00 41.33	A
	ATOM	1283	CD	GLU	180	28.262	30.958	93.945	1.00 42.95	A
	MOTA	1284	OE1		180	27.629	30.832	95.017	1.00 43.98	A
	MOTA	1285	OE2	GLU	180	29.174	31.798	93.795	1.00 44.03	A
60	MOTA	1286	С	GLU	180	28.147	26.241	92.048	1.00 32.62	A
	MOTA	1287	0	GLU	180	28.084	25.614	93.104	1.00 31.99	A
	MOTA	1288	N	ARG	181	28.706	25.745	90.951	1.00 30.63	A
	ATOM	1289	CA	ARG	181	29.292	24.415	90.941	1.00 30.51	A
	MOTA	1290	CB	ARG	181	29.050	23.739	89.587	1.00 34.25	A
65	MOTA	1291	CG	ARG	181	29.575	24.493	88.379		A
	ATOM	1292	CD	ARG	181	29.025	23.901	87.069	1.00 46.73	
										A
	ATOM	1293	NE	ARG	181	29.587	22.592	86.721	1.00 50.11	A
	MOTA	1294	CZ	ARG	181	30.818	22.400	86.251	1.00 52.44	A
	MOTA	1295	NH1	ARG	181	31.629	23.435	86.070	1.00 53.59	A
70	ATOM	1296	NH2		181	31.236	21.173	85.951	1.00 52.52	
										A
	MOTA	1297	c	ARG	181	30.781	24.480	91.249	1.00 28.82	A
	ATOM	1298	0	ARG	181	31.438	25.483	90.979	1.00 29.29	A
	ATOM	1299	N	LEU	182	31.308	23.408	91.829	1.00 25.57	A
									·	

	ATOM	1300	CA L	EU 18	2 32.718	23.348	92.1B2	1.00 21.92	A
	MOTA	1301		EU 18		22.553	93.471	1.00 20.02	A
	MOTA	1302		EU 18		23.087	94700	1.00 20.20	A
	ATOM	1303	CD1 L			22.044	95.812	1.00 17.99	A
5	ATOM	1304	CD2 L			24.379	95.159	1.00 16.82	Α
,	MOTA	1305		EU 18		22.696	91.069	1.00 22.08	A
				EU 18		21.949	90.257	1.00 19.82	A
	MOTA	1306					91.028	1.00 22.61	Ä
	MOTA	1307		ELN 18		23.000			A
10	MOTA	1308		LN 18		22.435	90.034	1.00 20.55	
10	MOTA	1309		LN 18		23.488	89.523	1.00 22.39	A
	MOTA	1310		LN 18		24.557	88.652	1.00 28.44	A
	MOTA	1311	CD G	IN 18		25.799	88.593	1.00 32.88	A
	MOTA	1312	OE1 G	IN 18		26.572	89.557	1.00 34.28	A
	ATOM	1313	NE2 G	SLN 18	3 37.664	25.989	87.468	1.00 33.10	A
15	ATOM	1314	CG	IN 18	3 36.518	21.327	90.702	1.00 19.22	A
	MOTA	1315	0 0	LN 18	3 36.795	21.390	91.897	1.00 18.40	A
	MOTA	1316	N P	1ET 18	4 36.902	20.330	89.915	1.00 18.69	A
	MOTA	1317	CA P	1ET 18	4 37.646	19.191	90.416	1.00 19.64	Α
	ATOM	1318		ÆT 18	4 36.747	17.951	90.361	1.00 21.90	A
20	MOTA	1319		ET 18		16.701	91.011	1.00 25.13	A
	MOTA	1320		TET 18		15.306	90.921	1.00 31.12	A
	ATOM	1321		ET 18		14.620	89.352	1.00 23.65	Α.
	MOTA	1322		TET 18		18.983	89.568	1.00 21.60	Α
	MOTA	1323		1ET 18		19.035	88.341	1.00 21.33	A
25	ATOM	1324		PHE 18		18.750	90.230	1.00 23.48	λ
23		1325		PHE 18		18.531	89.544	1.00 25.16	A
	MOTA	1326		PHE 18		19.736	89.709	1.00 25.59	A
	ATOM		-			21.064	89.414	1.00 25.42	A
	MOTA	1327					90.360	1.00 23.63	A
30	MOTA	1328	CD1 E			21.691	88.211	1.00 26.39	A
20	MOTA	1329	CD2 F			21.718		1.00 24.23	Ä
	MOTA	1330	CE1 E			22.956	90.124		
	MOTA	1331	CE2 F			22.987	87.961	1.00 27.17	A
	MOTA	1332		PHE 18		23.609	88.921	1.00 25.70	A
25.	MOTA	1333		PHE 18		17.326	90.149	1.00 26.03	A
35	MOTA	.1334		PHE 18		16.937	91.275	1.00 25.54	A
	MOTA	1335		ASP 18		16.743	89.414	1.00 29.33	A
	ATOM	1336		ASP 18		15.603	89.930	1.00 33.38	Α
	ATOM	1337	CB A	ASP 18		14.913	88.801	1.00 35.26	A
	ATOM	1338	CG 7	ASP 18	6 43.546	14.212	87.816	1.00 37.12	A
40	ATOM	1339	OD1 7	ASP 18	6 43.644	14.505	86.603	1.00 37.66	A
	ATOM	1340	OD2 I	ASP 18	6 42.733	13.368	88.257	1.00 36.31	A
	ATOM	1341	C 7	ASP 18	6 44.675	16.117	90:977	1.00 35.30	A
	MOTA	1342	0 7	ASP 18	6 45.167	17.238	90.865	1.00 35.53	A
	ATOM	1343		ASP 18	7 44.959	15.313	91.996	1.00 38.26	A
45	MOTA	1344		ASP 18		15.739	93.037	1.00 43.31	A
	ATOM	1345		ASP 18		15.138	94.385	1.00 42.12	A
	ATOM	1346		ASP 18		15.784	95.546	1.00 42.51	A
	ATOM	1347	OD1 A			15.631	96.696	1.00 42.87	A
	ATOM	1348	OD2 A			16.442	95.307	1.00 41.23	A
50	MOTA	1349		ASP 18		15.318	92.665	1.00 46.67	A
20		1350		ASP 18		14.138	92.719	1.00 48.15	A
	MOTA	1351				16.283	92.286	1.00 50.27	A
	MOTA			PRO 18		17.735	92.408	1.00 50.27	A
	MOTA	1352		PRO 18				1.00 53.10	Ä
55	MOTA	1353		PRO 18		15.996	91.897 91.561		A
22	MOTA	1354		PRO 18		17.376		1.00 52.20	
	MOTA	1355		PRO 18		18.263	92.503	1.00 52.65	A
	MOTA	1356		PRO 18		15.279	92.966	1.00 55.80	A
	MOTA	1357		PRO 18		14.568	92.650	1.00 56.91	Α.
	MOTA	1358	N A	ARG 18		15.466	94.228	1.00 58.59	A
60	ATOM	1359	CA A	ARG 18		14.812	95.321	1.00 61.67	A
	MOTA	1360	CB /	ARG 18	50.294	15.428	96.658	1.00 63.13	A
	MOTA	1361		ARG 18	50.839	16.823	96.881	1.00 65.91	A
	MOTA	1362		ARG 18		17.468	98.083	1.00 68.55	A
	ATOM	1363		ARG 18		17.670	97.855	1.00 70.63	A
65	ATOM	1364		ARG 18		18.095	98.784	1.00 72.05	A
	MOTA	1365	NH1				100.010	1.00 72.50	A
	MOTA	1366	NH2			18.252	98.484	1.00 72.44	A
	MOTA	1367		ARG 18		13.316	95.321	1.00 63.14	Ä
						12.537	94.652	1.00 63.21	Ä
70	ATOM	1368				12.537	96.070	1.00 64.30	Â
10	MOTA	1369		ASN 19				1.00 65.20	Ā
	MOTA	1370		ASN 19		11.509	96.140	1.00 65.20	A
	MOTA	1371		ASN 19		11.220	97.439		
	MOTA	1372	CG 1	ASN 19	00 47.172	12.273	97.753	1.00 67.73	A

	ATOM	1373	OD1	ASN	190	47.491	13.443	97.982	1.00 67.83	A
	MOTA	1374	ND2	asn	190	45.909	11.858	97.773	1.00 67.20	A
	MOTA	1375	Ç	asn	190	48.197	11.061	94.918	1.00 64.94	A
	MOTA	1376	0	ASN	190	47.182	11.662	94.565	1.00 64.53	A
5										
ر	MOTA	1377	N	LYS	191	48.669	9.999	94.273	1.00 64.72	A
	MOTA	1378	CA	LYS	191	48.018	9.463	93.083	1.00 63.98	A
	ATOM	1379	CB	LYS	191	48.810	8.266	92.541	1.00 65.18	A
	ATOM	1380	CG	LYS	191	48.799	7.041	93.447	1.00 66.13	A
	ATOM	1381	CD	LYS	191	49.405	5.830	92.747	1.00 67.02	A
10										
10	MOTA	1382	CE	LYS	191	49.274	4.572	93.593	1.00 68.29	A
	MOTA	1383	NZ	LYS	191	49.860	3.375	92.919	1.00 69.29	A
	ATOM	1384	С	LYS	191	46.577	9.039	93.358	1.00 62.26	A
	ATOM	1385	0	LYS	191	46.151	8.963	94.513	1.00 63.17	A
	MOTA	13B6	N	ARG	192	45.843	8.756	92.282	1.00 58.36	A
15	MOTA	1387	CA	ARG	192	44.440	8.350	92.348	1.00 54.26	A
13										
	MOTA	1388	CB	ARG	192	44.308	6.833	92.578	1.00 56.88	A
	MOTA	1389	CG	ARG	192	44.776	6.289	93.926	1.00 59.69	A
	MOTA	1390	CD	ARG	192	43.939	5.062	94.306	1.00 62.18	A
	MOTA	1391	NE	ARG	192	44.633	4.121	95.181	1.00 64.60	A
20	ATOM	1392	CZ	ARG	192	45.640	3.344	94.792	1.00 66.61	A
-0										
	MOTA	1393	NH1		192	46.074	3.400	93.539	1.00 66.97	A
	MOTA	1394	NH2	ARG	192	46.209	2.505	95.650	1.00 67.30	A
	MOTA	1395	С	ARG	192	43.619	9.106	93.391	1.00 50.08	A
~~	MOTA	1396	0	ARG	192	42.742	8.538	94.049	1.00 50.87	A
25	MOTA	1397	N	GLY	193	43.909	10.395	93.531	1.00 44.14	A
	MOTA	1398	CA	GLY	193	43.183	11.231	94.469	1.00 35.61	A
	MOTA	1399	C	·GLY	193	42.799	12.482	93.712	1.00 30.34	A
	MOTA	1400	0	GLY	193	43.343	12.732	92.639	1.00 30.32	A
20	MOTA	1401	N	VAL	194	41.865	13.264	94.238	1.00 25.49	A
30	ATOM	1402	CA	VAL	194	41.463	14.489	93.557	1.00 21.22	A
	ATOM	1403	CB	VAL	194	40.078	14.359	92.884	1.00 20.31	A
	MOTA	1404	CG1	VAL	194	40.100	13.289	91.809	1.00 19.29	A
	ATOM	1405	CG2	VAL	194	39.032	14.059	93.935	1.00 18.96	A
	ATOM	1406	С	VAL	194	41.375	15.66B	94.505	1.00 20.08	A
25										
35	MOTA	1407	0	VAL	194	41.417	15.515	95.722	1.00 20.27	A
	MOTA	1408	N	ILE	195	41.238	16.853	93.930	1.00 20.12	A
	ATOM	1409	CA		195					A
				ILE		41.109	18.065	94.713	1.00 18.57	
	MOTA	1410	CB	ILE	195	42.298	19.014	94.477	1.00 20.69	A
	MOTA	1411	CG2	ILE	195	42.011	20.362	95.118	1.00 21.74	A
40	ATOM	1412								
70			CG1		195	43.584	18.392	95.029	1.00 21.99	Α
	ATOM	1413	CD1	ILE	195	44.853	19.212	94.722	1.00 23.27	A
	MOTA	1414	С	ILE	195	39.838	18.791	94.297	1.00 17.41	A
	MOTA	1415	0	ILE	195	39.639	19.077	93.115	1.00 15.50	A
	MOTA	1416	N	ILE	196	38.962	19.066	95.256	1.00 17.01	A
45	ATOM	1417	CA	ILE	196	37.751	19.805	94.939	1.00 18.54	A
	MOTA	1418	CB	ILE	196	36.493	19.251	95.639	1.00 18.28	A
	MOTA	1419	CG2	ILE	196	35.299	20.143	95.314	1.00 13.69	A
	ATOM	1420	CG1		196	36.209	17.819	95.171	1.00 17.38	A
	MOTA	1421	CD1	ILE	196	37.016	16.775	95.894	1.00 21.62	A
50	ATOM	1422	С	ILE	196	37.981	21.232	95.407	1.00 20.22	A
	ATOM	1423	0	ILE	196	38.001	21.517	96.606	1.00 20.32	Α
	MOTA	1424	N	LYS	197	38.158	22.122	94.441	1.00 21.72	A
	MOTA	1425	CA	LYS	197	38.418	23.524	94.709	1.00 23.72	A
	ATOM	1426	CB	LYS	197	38.807	24.209	93.397	1.00 26.40	A
55										
JJ	MOTA	1427	CG	LYS	197	39.068	25.693	93.481	1.00 29.01	A
	ATOM	1428	CD	LYS	197	39.519	26.211	92.125	1.00 32.62	A
	ATOM	1429	ÇE	LYS	197	39.538	27.728	92.088	1.00 33.50	A
	MOTA	1430	NZ	LYS	197	38.172	28.259	92.341	1.00 36.03	A
	ATOM	1431	С	LYS	197	37.226	24.225	95.348	1.00 24.04	Α
60										
00	ATOM	1432	0	LYS	197	36.139	24.261	94.782	1.00 24.54	A
	MOTA	1433	N	GLY	198	37.436	24.763	96.543	1.00 24.46	A
	MOTA	1434	CA	GLY	198	36.377				
							25.478	97.227	1.00 25.68	A
	MOTA	1435	С	GLY	198	35.413	24.681	98.088	1.00 26.82	A
	MOTA	1436	0	GLY	198	34.482	25.256	98.652	1.00 27.32	A
65										
O)	MOTA	1437	N	LEU	199	35.612	23.373	98.202	1.00 27.36	A
	ATOM	1438	CA	LEU	199	34.714	22.558	99.017	1.00 27.19	A
	MOTA	1439	CB	LEU	199	35.008				
							21.068	98.819	1.00 26.21	A
	ATOM	1440	CG	LEU	199	33.908	20.008	99.023	1.00 27.04	A
	ATOM	1441	CD1		199	34.563	18.778	99.630	1.00 25.53	A
70										
,,,	ATOM	1442	CD2		199	32.779	20.497	99.924	1.00 24.18	A
	MOTA	1443	C	LEU	199	34.920	22.925	100.484	1.00 27.51	A
	ATOM	1444	ō	LEU	199	36.024		101.005	1.00 28.57	A
	MOTA	1445	N	GLU	200	33.856	23.346	101.150	1.00 28.60	A

	MOTA	1446	CA	GLU	200	33.950	23.721	102.553	1.00 31.25	Α
	MOTA	1447	CB	GLU	200	32.788	24.644	102.935	1.00 34.22	A
	ATOM	1448	CG	GLU	200	32.933	26.067	102.419	1.00 39.68	A
	MOTA	1449	CD	GLU	200	34.051	26.823	103.108	1.00 42.07	A
5	ATOM	1450		GLU	200	33.921		104.317	1.00 44.27	Ä
_	ATOM	1451		GLU	200	35.065		102.443	1.00 44.71	Ä
	MOTA	1452							1.00 30.44	
			C	GLU	200	33.986		103.516		A
	MOTA	1453	0	GLU	200	33.381		103.282	1.00 28.54	A
10	MOTA	1454	N	GLU	201	34.716		104.606	1.00 30.76	A
10	MOTA	1455	CA	GLU	201	34.841	21.730	105.649	1.00 29.99	A
	MOTA	1456	CB	GLU	201	36.281	21.247	105.742	1.00 29.82	Α
	MOTA	1457	CG	GLU	201	36.755	20.516	104.511	1.00 32.15	A
	ATOM	1458	CD	GLU	201	38.156		104.676	1.00 35.25	A
	MOTA	1459		GLU	201	38.408		105.699	1.00 34.69	A
15	ATOM	1460							1.00 36.53	
13				GLU	201	39.000		103.786		A
	ATOM	1461	C	GLU	201	34.439		106.943	1.00 29.40	A
	MOTA	1462	0	GLU	201	35.183		107.465	1.00 30.31	A
	MOTA	1463	N	ILE	202	33.256	22.089	107.449	1.00 27.91	A
	ATOM	1464	CA	ILE	202	32.765	22.694	108.679	1.00 25.94	A
20	MOTA	1465	CB	ILE	202	31.207	22.720	108.720	1.00 27.58	A
	MOTA	1466	CG2	ILE	202	30.721		110.096	1.00 24.19	A
	ATOM	1467		ILE	202	30.662		107.682	1.00 28.28	Ä.
	MOTA	1468		ILE	202	30.809		106.256	1.00 30.78	A
	MOTA	1469	C			33.277				
25				ILE	202			109.889	1.00 25.41	. y
23	MOTA	1470	0	ILE	202	33.195		109.945	1.00 25.37	A
	MOTA	1471	N	THR	203	33.811		110.856	1.00 23.88	A
	MOTA	1472	CA	THR	203	34.321	22.070	112.083	1.00 22.88	A
	MOTA	1473	CB	THR	203	35.397	22.981	112.742	1.00 22.77	A
	MOTA	1474	OG1	THR	203	36.542	23.064	111.883	1.00 23.19	A
30	ATOM	1475		THR	203	35.813		114.112	1.00 19.08	A
	MOTA	1476	c	THR	203	33.143		113.038	1.00 22.21	A
	MOTA	1477	ŏ	THR	203	32.385		113.242	1.00 22.47	A
	MOTA	1478	N	VAL	204	32.977		113.606	1.00 21.39	A
25.	MOTA	1479	CA	VAL	204	31.891		114.549	1.00 21.47	A
35	MOTA	1480	CB	VAL	204	31.248		114.278	1.00 20.28	A
	MOTA	1481	CG1	VAL	204	30.034	18.906	115.162	1.00 21.96	A
	MOTA	1482	CG2	VAL	204	30.859	19.000	112.820	1.00 20.66	A
	MOTA	1483	С	VAL	204	32.531	20,490	115.939	1.00 23.52	A
	MOTA	1484	0	VAL	204	33.083		116.385	1.00 24.43	A
40	MOTA	1485	N	HIS	205	32.468		116.615	1.00 23.51	A
	MOTA	1486	CA	HIS	205	33.088		117.933	1.00 24.78	A
	MOTA	1487	СВ							
				HIS	205	32.979		118.407	1.00 24.16	A
	MOTA	1488	CG	HIS	205	33.597		117.460	1.00 28.16	A
15	MOTA	1489		HIS	205	34.887		117.281	1.00 28.25	A
45	MOTA	1490		HIS	205	32.870	24.885	116.493	1.00 29.05	A
	ATOM	1491	CE1	HIS	205	33.684	25.623	115.759	1.00 27.33	A
	MOTA	1492	NE2	HIS	205	34.914	25.464	116.216	1.00 28.33	A
	MOTA	1493	С	HIS	205	32.586	20.836	119.018	1.00 24.15	A
	ATOM	1494	0	HIS	205	33.341		119.909	1.00 24.11	A
50	ATOM	1495	N	ASN	206	31.318		118.945	1.00 25.62	A
	MOTA	1496	CA	ASN	206	30.758		119.939	1.00 26.43	Ä
	MOTA	1497	CB							
				ASN	206	30.598		121.281	1.00 25.52	A
	ATOM	1498	CG	ASN	206	29.689		121.186	1.00 26.18	A
55	MOTA	1499		ASN	. 206	28.498	21358	120.906	1.00 28.63	A
55	MOTA	1500	ND2	ASN	. 206	30.246	22.671	121.414	1.00 24.14	A
	MOTA	1501	С	ASN	206	29.422	18.960	119.496	1.00 27.20	· A
	MOTA	1502	0	ASN	206	28.804		118.533	1.00 27.37	A
	ATOM	1503	N	LYS	207	28.993		120.212	1.00 27.93	A
	MOTA	1504	CA	LYS	207	27.751		119.924	1.00 30.13	A
60	ATOM	1505	CB.	LYS	207					
00	_		~~			27.449		121.060	1.00 32.58	A
	MOTA	1506	CG	LYS	207	26,151		120.906	1.00 36.84	A
	MOTA	1507	CD	LYS	207	25.112		121.929	1.00 40.39	A
	MOTA	1508	CE	LYS	207	25.525	15.543	123.349	1.00 41.61	A
	MOTA	1509	NZ	LYS	207	24.489	15.948	124.350	1.00 43.85	A
65	MOTA	1510	С	LYS	207	26.571		119.725	1.00 29.76	λ
	MOTA	1511	ō	LYS	207	25.738		118.850	1.00 30.05	Ä
	ATOM	1512	N	ASP	208	26.505		120.523	1.00 28.95	
	ATOM	1513	CA							A
				ASP	208	25.402		120.429	1.00 27.71	A
70	MOTA	1514	CB	ASP	208	25.280		121.751	1.00 28.92	A
70	MOTA	1515	CG	ASP	208	24.772		122.895	1.00 33.21	λ
	MOTA	1516		ASP	208	24.967	20.444	124.081	1.00 32.92	A
	MOTA	1517	OD2	ASP	208	24.165	19.037	122.609	1.00 34.60	A
	MOTA	1518	С	ASP	208	25.524		119.240	1.00 26.33	A
									· -	

		1510	_						
	MOTA	1519	0	ASP	208	24.836	22.186 119.156	1.00 26.39	Α
	MOTA	1520	N	GLU	209	26.381	20.810 118.296	1.00 24.27	A
	ATOM	1521	CA	GLU	209	26.580	21.630 117.116	1.00 21.87	A
	MOTA	1522	СВ	GLU	209	28.039	22.074 117.066	1.00 23.60	Ä
5	MOTA	1523	CS	GLU	209	28.331			
-							23.202 116.106	1.00 25.30	A
	MOTA	1524	CD	GLU	209	29.678	23.849 116.384	1.00 25.66	A
	MOTA	1525		GLU	209	29.872	24.362 117.507	1.00 25.63	A
	MOTA	1526	OE2	GLU	209	30.538	23.845 115.481	1.00 26.97	A
	ATOM	1527	С	GLU	209	26.217	20.819 115.874	1.00 19.67	A
10	ATOM	1528	0	GLU	209	26.125	21.350 114.769	1.00 18.53	A
	ATOM	1529	N	VAL	210	25.988			
	MOTA						19.528 116.075	1.00 16.60	A
		1530	CA	VAL	210	25.648	18.625 114.985	1.00 17.06	A
	MOTA	1531	CB	VAL	210	25.654	17.148 115.479	1.00 17.27	A
1.5	MOTA	1532	CG1	VAL	210	25.307	16.224 114.330	1.00 18.17	A
15	MOTA	1533	CG2	VAL	210	27.028	16.779 116.068	1.00 17.55	A
	MOTA	1534	С	VAL	210	24.305	18.895 114.270	1.00 16.45	A
	MOTA	1535	. 0	VAL	210	24.267	19.119 113.063	1.00 17.67	. A
	ATOM	1536	N	TYR	211	23.203	18.882 115.003	1.00 14.85	A
	ATOM	1537	CA	TYR	211	21.911			
20							19.072 114.366	1.00 15.99	A
20	MOTA	1538	CB	TYR	211	20.789	19.050 115.404	1.00 14.76	A
	MOTA	1539	CG	TYR	211	19.431	18.850 114.780	1.00 14.73	A
	MOTA	1540	CD1		211	19.179	17.755 113.953	1.00 12.63	A
	ATOM	1541	CE1	TYR	211	17.923	17.557 113.387	1.00 14.15	A
	MOTA	1542	CD2	TYR	211	18.395	19.746 115.025	1.00 15.52	A
25	MOTA	1543	CE2		211	17.136	19.559 114.466	1.00 16.40	· A
	MOTA	1544	cz	TYR	211	16.903			
	ATOM	1545	ОН	TYR		15.645	18.462 113.649	1.00 15.49	Α.
					211		18.271 113.116	1.00 12.99	A
	ATOM	1546	C	TYR	211	21.763	20.303 113.483	1.00 15.43	A
20	MOTA	1547	0	TYR	211	21.220	20.207 112.383	1.00 17.14	A
30	ATOM	1548	N	GLN	212	22.238	21.456 113.925	1.00 15.05	A
	ATOM	1549	CA	GLN	212	22.080	22.624 113.081	1.00 17.00	λ
	ATOM	1550	CB	GLN	212	22.384	23.912 113.855	1.00 18.93	A
	MOTA	1551	CG	GLN	212	23.803	24.099 114.319	1.00 25.15	A
	ATOM	1552	CD	GLN	212	23.892	25.178 115.379		
35	ATOM	1553						1.00 29.02	A
23			OE1		212	23.354	26.276 115.209	1.00 30.43	A
	MOTA	1554		GLN	212	24.562	24.870 116.486	1.00 30.19	A
	MOTA	1555	С	GLN	212	22.903	22.543 111.799	1.00 16.71	A
	MOTA	1556	0	GLN	212	22.459	23.030 110.749	1.00 16.05	A
4.0	MOTA	1557	N	ILE	213	24.077	21.913 111.865	1.00 14.80	A
40	MOTA	1558	CA	ILE	213	24.921	21.776 110.678	1.00 13.74	A
	MOTA	1559	CB	ILE	213	26.309	21.148 111.036	1.00 14.83	A
	MOTA	1560		ILE	213	27.118	20.846 109.764		
	ATOM	1561		ILE	213			1.00 11.99	A
						27.099	22.122 111.926	1.00 13.49	A
45	ATOM	1562		ILE	213	28.495	21.607 112.366	1.00 12.70	A
40	MOTA	1563	С	ILE	213	24.170	20.909 109.662	1.00 14.25	A
	MOTA	1564	0	ILE	213	24.135	21.223 108.474	1.00 14.16	A
	MOTA	1565	N	LEU	214	23.546	19.838 110.142	1.00 12.87	A
	ATOM	1566	CA	LEU	214	22.778	18.968 109.273	1.00 13.78	A
	ATOM	1567	CB	LEU	214	22.355	17.705 110.022	1.00 11.53	A
50	ATOM	1568	CG	LEU	214	23.467	16.843 110.623	1.00 10.45	A
	ATOM	1569		LEU	214	22.840			
	ATOM	1570		LEU				1.00 10.08	A
					214	24.454	16.418 109.552	1.00 9.12	A
	MOTA	1571	C	LEU	214	21.536	19.695 108.749	1.00 16.52	A
55	ATOM	1572	0	LEU	214	21.172	19.527 107.591	1.00 19.62	A
55	ATOM	1573	N	GLU	215	20.881	20.495 109.590	1.00 16.71	A
	MOTA	1574	CA	GLU	215	19.690	21.239 109.152	1.00 19.78	A
	ATOM	1575	CB	GLU	215	19.085	22.053 110.306	1.00 19.90	A
	MOTA	1576	CG	GLU	215	18.435	21.249 111.418	1.00 21.54	Ä
	MOTA	1577	CD	GLU	215	17.901	22.154 112.513	1.00 24.54	
60	ATOM	1578		GLU		16.661			A
-	ATOM	1579			215		22.267 112.659	1.00 25.81	A
				GLU	215	18.728	22.768 113.219	1.00 23.71	A
	ATOM	1580	С	GLU	215	20.049	22.211 108.025	1.00 20.52	A
	MOTA	1581	0	GLU	215	19.311	22.361 107.048	1.00 19.08	A
	MOTA	1582	N	LYS	216	21.189	22.878 108.189	1.00 21.26	A
65	MOTA	1583	CA	LYS	216	21.677	23.840 107.215	1.00 22.33	Ä
	ATOM	1584	CB	LYS	216	23.046	24.367 107.656	1.00 24.51	
	MOTA	1585	CG	LYS	216	23.510			A
	ATOM	1586					25.619 106.938	1.00 28.98	A
			CD	LYS	216	22.872	26.865 107.523	1.00 33.02	A
70	MOTA	1587	CE	LYS	216	23.331	27.078 108.959	1.00 35.90	A
70	ATOM	1588	NZ	LYS	216	24.819	27.142 109.072	1.00 37.29	A
	ATOM	1589	¢	LYS	216	21.782	23.150 105.850	1.00 22.36	. , A
	MOTA	1590	0	LYS	216	21.371	23.708 104.832	1.00 23.95	A
	MOTA	1591	N	GLY	217	22.318	21.931 105.838	1.00 20.62	A
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	ATOM	1592	CA	GLY	217	22.458	21.193	104.595	1.00 19.15	A
	ATOM	1593	С	GLY	217	21.119	20.836	103.976	1.00 19.07	A
	ATOM	1594	0	GLY	217	20.938		102.760	1.00 18.70	A
	MOTA	1595	N	ALA	218	20.168		104.812	1.00 17.10	A
- 5	ATOM	1596	CA	ALA	218				1.00 15.84	A
,						18.845		104.330		
	ATOM	1597	CB	ALA	218	17.996		105.471	1.00 14.05	A
	MOTA	1598	С	ALA	218	18.157		103.696	1.00 15.48	A
	ATOM	1599	0	ALA	218	17.533	21.155	102.638	1.00 15.90	A
_	ATOM	1600	N	ALA	219	18.273	22.436	104.331	1.00 14.41	A
10	MOTA	1601	CA	ALA	219	17.638		103.800	1.00 14.13	A
	ATOM	1602	CB	ALA	219	17.776		104.787	1.00 12.71	A
	MOTA	1603		ALA	219	18.208		102.452	1.00 13.46	A
	MOTA	1604	0	ALA	219	17.469		101.561	1.00 13.70	A
	MOTA	1605	N	LYS	220	19.525		102.304	1.00 13.95	A
15	ATOM	1606	CA	LYS	220	20.146	24.357	101.045	1.00 14.23	A
	ATOM	1607	CB	LYS	220	21.666	24.380	101.192	1.00 12.72	A
	MOTA	1608	CG	LYS	220	22.360	25.077	100.038	1.00 17.07	A
	MOTA	1609	CD	LYS	220	23.833		100.309	1.00 15.93	A
	ATOM	1610	CE	LYS	220	24.512	25.923	99.080	1.00 17.58	A
20	ATOM	1611			220				1.00 15.01	Ä
20			NZ	LYS		25.991	26.097	99.261		
	ATOM	1612	C	LYS	220	19.718	23.360	99.969	1.00 14.89	A
	MOTA	1613	0	LYS	220	19.497	23.722	98.809	1.00 15.14	A.
	ATOM	1614	N	ARG	221	19.572	22.105	100.380	1.00 14.35	A
	MOTA	1615	CA	ARG	221	19.166	21.024	99.492	1.00 15.09	A
25	ATOM	1616	CB	ARG	221	19.185	19.714	100.274	1.00 14.48	A
	MOTA	1617	CG	ARG	221	19.467	18.488	99.455	1.00 18.77	A
	MOTA	1618	CD	ARG	221	19.485		100.365	1.00 20.34	A
		1619								
	ATOM		NE	ARG	221	20.806		100.446	1.00 21.59	A
20	MOTA	1620	CZ	ARG	221	21.148		101.357	1.00 21.60	A
30	MOTA	1621		ARG	221	20.264		102.272	1.00 19.86	A
	MOTA	1622	NH2	ARG	221	22.367	15.218	101.344	1.00 19.97	A
	MOTA	1623	С	ARG	221	17.761	21.290	98.932	1.00 15.56	A
•	ATOM	1624	0	ARG	221	17.419	20.858	97.827	1.00 15.28	A
	ATOM	1625	N	THR	222	16.945	22.004	99.698	1.00 14.05	A
35	MOTA	1626	CA	THR	222	15.608	22.325	99.253	1.00 13.31	A
55	MOTA	1627	CB	THR	222			100.384	1.00 16.22	Ä
						14.781				
	MOTA	1628		THR	222	14.707	22.058	101.495	1.00 16.19	A
	MOTA	1629	CG2		222	13.367	23.252	99.904	1.00 17.44	A
40	MOTA	1630	С	THR	222	15.679	23.284	98.061	1.00 13.31	A
40	MOTA	1631	0	THR	222	14.850	23.205	97.156	1.00 12.26	A
	ATOM	1632	N	THR	223	16.667	24.175	98.044	1.00 11.79	A
	ATOM	1633	CA	THR	223	16.787	25.112	96.936	1.00 13.70	A
	ATOM	1634	CB	THR	223	17.675	26.345	97.287	1.00 14.50	A
	MOTA	1635		THR	223	19.058	25.979	97.247	1.00 18.73	A
45		1636		THR	223					λ
43	MOTA					17.343	26.870	98.669	1.00 10.63	
	MOTA	1637	C	THR	223	17.387	24.398	95.729	1.00 15.22	λ
	MOTA	1638	0	THR	223	17.148	24.778	94.580	1.00 17.54	A
	MOTA	1639	N	ALA	224	18.176	23.361	95.986	1.00 14.46	A
	MOTA	1640	CA	ALA	224	18.773	22,607	94.896	1.00 13.62	A
50	MOTA	1641	CB	ALA	224	19.793	21.615	95.432	1.00 14.83	A
	MOTA	1642	С	ALA	224	17.665	21.867	94.171	1.00 13.10	A
	MOTA	1643	0	ALA	224	17.672	21.775	92.958	1.00 13.24	A
	MOTA	1644	N	ALA	225	16.710	21.346	94.932	1.00 13.91	A
		1645	CA	ALA	225		20.596	94.369	1.00 15.07	λ
55	MOTA					15.598				
55	MOTA	1646	CB	ALA	225	14.817	19.903	95.498	1.00 15.97	A
	MOTA	1647	C	ALA	225	14.640	21.422	93.498	1.00 14.78	A
	MOTA	1648	0	ALA	225	14.070	20.908	92.532	1.00 13.24	A
	MOTA	1649	N	THR	226	14.449	22.694	93.822	1.00 15.56	A
	ATOM	1650	CA	THR	226	13.555	23.490	92.995	1.00 16.82	A
60	ATOM	1651	CB	THR	226	12.992	24.729	93.747	1.00 17.66	A
	MOTA	1652		THR	226	13.314	25.921	93.015	1.00 21.16	A
	MOTA	1653		THR	226	13.557	24.822	95.142	1.00 16.64	A
	MOTA	1654	Ç	THR	226	14.300	23.943	91.745	1.00 15.61	A
45	MOTA	1655	0	THR	226	13.685	24.257	90.726	1.00 13.81	A
65	ATOM	1656	N	LEU	227	15.629	23.947	91.828	1.00 14.58	A
	ATOM	1657	CA	LEU	227	16.473	24.361	90.716	1.00 14.64	A
	MOTA	1658	CB	LEU	227	17.751	24.993	91.267	1.00 17.19	A
	ATOM	1659	CG	LEU	227	18.827	25.459	90.285	1.00 22.76	A
	MOTA	1660		LEU	227	18.209	26.283	89.160	1.00 21.40	λ
70		1661								
10	ATOM			LEU	227	19.873	26.272	91.055	1.00 24.08	A
	MOTA	1662	C	LEU	227	16.808	23.223	89.742	1.00 15.20	A
	ATOM	1663	0	LEU	227	16.939	23.453	88.540	1.00 16.19	A
	MOTA	1664	N	MET	228	16.924	22.000	90.256	1.00 13.63	A

	MOTA	1665	CA	MET	228	17.244	20.842	89.424	1.00 14.22	A
	ATOM	1666	СВ	MET	228	18.607	20.275	89.852	1.00 17.08	A
	ATOM	1667	CG	MET	228	19.771	21.243	89.583	1.00 18.22	Ä
				MET	228			90.414	1.00 19.64	Ä
5	MOTA	1668	SD			21.340	20.816	91.964	1.00 16.95	À
,	MOTA	1669	CE	MET	228	21.189	21.761			
	ATOM	1670	C	MET	228	16.148	19.768	89.504	1.00 13.11	A
	MOTA	1671	0	MET	228	15.683	19.423	90.588	1.00 10.34	A
	ATOM	1672	N	ASN	229	15.748	19.243	88.348	1.00 12.86	λ
• •	MOTA	1673	CA	ASN	229	14.676	18.246	88.259	1.00 13.74	A
10	ATOM	1674	CB	ASN	229	14.319	17.975	86.794	1.00 13.77	A
	ATOM	1675	CG	ASN	229	13.993	19.241	86.023	1.00 15.98	A
	MOTA	1676	OD1	NZA	229	13.899	19.221	84.790	1.00 16.80	A
	MOTA	1677	ND2	ASN	229	13.814	20.352	86.740	1.00 15.44	A
	ATOM	1678	С	ASN	229	14.976	16.915	88.930	1.00 14.79	A
15	MOTA	1679	0	ASN	229	16.036	16.322	88.713	1.00 15.96	A
	MOTA	1680	N	ALA	230	14.022	16.444	89.728	1.00 12.65	A
	MOTA	1681	CA	ALA	230	14.155	15.182	90.443	1.00 13.20	A
	MOTA	1682	CB	ALA	230	13.971	14.010	89.476	1.00 11.65	A
	MOTA	1683	C	ALA	230	15.514	15.099	91.114	1.00 12.14	A
20	MOTA	1684	0	ALA	230	16.187	14.071	91.056	1.00 11.89	A
	MOTA	1685	N	TYR	231	15.906	16.190	91.753	1.00 11.37	A
	MOTA	1686	CA	TYR	231	17.190	16.270	92.435	1.00 12.67	A
	MOTA	1687	СВ	TYR	231	17.325	17.625	93.128	1.00 13.10	A
	MOTA	1688	CG	TYR	231	18.685	17.843	93.720	1.00 13.58	A
25	ATOM	1689		TYR	231	18.951	17.526	95.050	1.00 15.59	A
23	MOTA	1690			231	20.235	17.687	95.583	1.00 15.33	Ä
			CE1	TYR	231		18.325	92.934	1.00 14.58	Ä
	MOTA	1691		TYR		19.728 21.008			1.00 15.62	Ä
	ATOM	1692	CE2		231		18.489	93.454		
30	MOTA	1693	CZ	TYR	231	21.251	18.169	94.777	1.00 14.53	A
20	MOTA	1694	ОН	TYR	231	22.508	18.355	95.291	_	A
	MOTA	1695	C	TYR	231	17.431	15.162	93.458	1.00 12.52	A
	MOTA	1696	0	TYR	231	18.470	14.500	93.436	1.00 12.31	A
	MOTA	1697	N	SER	232	16.457	14.968	94.341	1.00 12.51	Α
25	MOTA	1698	CA	SER	232	16.543	13.978	95.406	1.00 11.76	A
35	ATOM	1699	CB	SER	232	15.325	14.091	96.331	1.00 10.64	A
	MOTA	1700	OG	SER	232	14.143	13.654	95.692	1.00 10.59	A
	MOTA	1701	С	SER	232	16.691	12.534	94.936	1.00 12.25	A
	ATOM	1702	0	SER	232	17.123	11.673	95.702	1.00 12.40	A
	ATOM	1703	N	SER	233	16.332	12.244	93.695	1.00 11.36	A
40	MOTA	1704	CA	SER	233	16.485	10.876	93.241	1.00 12.78	A
	ATOM	1705	CB	SER	233	15.146	10.341	92.712	1.00 13.58	A
	MOTA	1706	OG	SER	233	. 14.735	11.011	91.547	1.00 17.87	A
	ATOM	1707	С	SER	233	17.598	10.719	92.199	1.00 12.96	. A
	ATOM	1708	0	SER	233	18.129	9.628	92.018	1.00 12.33	Ά
45	MOTA	1709	N	ARG	234	17.984	11.817	91.552	1.00 13.08	A
	ATOM	1710	CA	ARG	234	19.022	11.770	90.519	1.00 12.98	A
	MOTA	1711	CB	ARG	234	18.639	12.658	89.333	1.00 13.88	A
	ATOM	1712	CG	ARG	234	17.411	12.209	88.575	1.00 15.89	A
	ATOM	1713	CD	ARG	234	17.135	13.146	87.408	1.00 16.18	A
50	ATOM	1714	NE	ARG	234	15.961	12.713	86.672	1.00 20.62	A
	ATOM	1715	CZ	ARG	234	15.330	13.442	85.761	1.00 21.81	A
	ATOM	1716		ARG	234	15.764	14.662	85.459	1.00 21.30	λ
	ATOM	1717		ARG	234	14.249	12.951	85.168	1.00 21.53	Ä
	MOTA	1718	C	ARG	234	20.409	12.182	90.972	1.00 11.75	Ä
55					234	21.374	12.011	90.230	1.00 11.05	Ä
<i>J J</i>	MOTA	1719	0	ARG				92.170	1.00 9.69	
	MOTA	1720	N	SER	235	20.510	12.744			A
	MOTA	1721	CA	SER	235	21.802	13.185	92.679	1.00 9.62	A
	ATOM	1722	CB	SER	235	21.656	14.525	93.409	1.00 9.37	A
60	MOTA	1723	OG	SER	235	20.858	14.410	94.575	1.00 9.00	A
oo	MOTA	1724	С	SER	235	22.445	12.171	93.617	1.00 9.66	A
	MOTA	1725	0	SER	235		11.317	94.190	1.00 12.40	λ
	ATOM	1726	N	HIS	236	23.762	12.287	93.758	1.00 8.64	A
	MOTA	1727	CA	HIS	236	24.573	11.436	94.627	1.00 5.39	A
c=	MOTA	1728	CB	HIS	236	25.795	10.898	93.878	1.00 6.60	Α
65	MOTA	1729	CG	HIS	236	25.474	10.085	92.666	1.00 6.36	A
	MOTA	1730		HIS	236	25.516	10.398	91.350	1.00 6.40	A
	MOTA	1731	ND1	HIS	236	25.109	8.758	92.732	1.00 6.26	A
	MOTA	1732		HIS	236	24.945	8.287	91.509	1.00 4.95	A
	MOTA	1733	NE2	HIS	236	25.186	9.261	90.652	1.00 5.93	A
70	MOTA	1734	С	HIS	236	25.092	12.348	95.732	1.00 6.58	A
	ATOM	1735	0	HIS	236	25.676	13.396	95.446	1.00 5.89	A
	MOTA	1736	N	SER	237	24.902	11.972	96.990	1.00 7.32	A
	ATOM	1737	CA	SER	237	25.409	12.816	98.063	1.00 7.91	A

	N/MOV	1720	CD	CED	237	24.287	12 204	99.022	1.00 8.40	A
	MOTA	1738	CB	SER			13.204		1.00 12.48	A
	MOTA	1739	0G	SER	237	23.895	12.093	99.805		
	ATOM	1740	C	SER	237	26.505	12.089	98.830	1.00 7.51	A
_	MOTA	1741	0	SER	237	26.365	10.916	99.179	1.00 10.56	A
5	ATOM	1742	N	VAL	238	27.593	12.794	99.092	1.00 7.01	A
	MOTA	1743	CA	VAL	238	28.714	12.236	99.822	1.00 7.37	A
	MOTA	1744	CB	VAL	238	30.032	12.305	98.998	1.00 8.80	A
	MOTA	1745	CG1	VAL	238	31.145	11.578	99.741	1.00 6.78	A
	MOTA	1746	CG2	VAL	238	29.833	11.711	97.603	1.00 5.26	A
10	MOTA	1747	С	VAL	238	28.938	13.025	101.107	1.00 8.29	A
	MOTA	1748	0	VAL	238	29.445	14.141 3	101.057	1.00 8.87	A
	MOTA	1749	N	PHE	239	28.549	12.454 1		1.00 7.65	A
	ATOM	1750	CA	PHE	239	28.756	13.114 1		1.00 7.41	A
	MOTA	1751	CB	PHE	239	27.557	12.895		1.00 7.34	A
15	ATOM	1752	CC	PHE	239	27.615	13.694		1.00 6.91	A
13	ATOM	1753		PHE	239	28.508	13.355		1.00 7.70	A
		1754		PHE	239	26.778	14.788		1.00 6.68	A
	MOTA								1.00 7.54	Ä
	MOTA	1755		PHE	239	28.567	14.102			Â
20	MOTA	1756			239	26.828	15.546 1			
20	ATOM	1757	CZ	PHE	239	27,.724	15.201 1		1.00 7.57	A
	MOTA	1758	C	PHE	239	30.016	12.525		1.00 10.17	A
	MOTA	1759	0	PHE	239	30.063	11.334		1.00 10.87	Α.
	MOTA	1760	N	SER	240	31.036	13.356		1.00 9.89	A
0.5	MOTA	1761	CA	SER	240	32.283	12.893		1.00 11.46	A
25	MOTA	1762	CB	SER	240	33.441	13.168		1.00 10.05	A
	MOTA	1763	OG	SER	240	33.183	12.621	102.681	1.00 14.59	A
	MOTA	1764	С	SER	240	32.598	13.508	106.285	1.00 12.92	A
	MOTA	1765	0	SER	240	32:405	14.705	106.509	1.00 12.61	Α
	MOTA	1766	N	VAL	241	33.078	12.665	107.193	1.00 12.52	Α
30	MOTA	1767	CA	VAL	241	33.468	13.113 1	108.511	1.00 13.59	A
	MOTA	1768	CB	VAL	241	32.559	12.501		1.00 14.83	A
	ATOM	1769		VAL	241	32.526	10.991		1.00 17.21	A
	MOTA	1770		VAL	241	33.054	12.922		1.00 13.88	A
	MOTA	1771	c	VAL	241	34.931	12.718		1.00 13.59	A
35	MOTA	1772	ŏ	VAL	241	35.305	11.548		1.00 10.71	Α
55			N	THR	242	35.759	13.715		1.00 14.44	Ä
	MOTA	1773								Ä
	MOTA	1774	CA	THR	242	37.175	13.489		1.00 15.80	
	ATOM	1775.	CB	THR	242	38.051	14.421		1.00 16.64	A
40	MOTA	1776		THR	242	37.719	14.238		1.00 19.41	A
40	MOTA	1777		THR	242	39.539	14.102		1.00 11.48	A
	MOTA	1778	C	THR	242	37.479	13.726		1.00 17.79	A
	MOTA	1779	0	THR	242	37.051	14.719		1.00 19.50	A
	MOTA	1780	N	ILE	243	38.224	12.805		1.00 18.66	A
4.5	MOTA	1781	CA	ILE	243	38.563	12.904		1.00 20.82	A
45	MOTA	1782	CB	ILE	243	37.972	11.714	113.500	1.00 20.34	A
	MOTA	1783	CG2	ILE	243	38.085	11.953	114.993	1.00 20.79	A
	MOTA	1784	CG1	ILE	243	36.506	11.524	113.114	1.00 21.41	A
	MOTA	1785	CD1	ILE	243	35.902	10.213	113.632	1.00 20.85	Α
	MOTA	1786	C	ILE	243	40.076	12.928	112.958	1.00 23.56	A
50	ATOM	1787	ò	ILE	243	40.782	11.953		1.00 23.06	A
	ATOM	1788	N	HIS	244	40.574	14.053		1.00 25.26	A
	ATOM	1789	CA	HIS	244 .	41.994	14.177		1.00 27.63	A
	MOTA	1790	CB	HIS	244	42.507	15.589		1.00 28.72	A
	MOTA	1791	CG	HIS	244	42.974	15.799		1.00 32.69	A
55	ATOM	1792		HIS	244	44.219	15.803		1.00 33.88	Ä
23		1793				42.111	16.067		1.00 34.05	A
	MOTA			HIS	244					
	MOTA	1794		HIS	244	42.803	16.231		1.00 33.87	A
	MOTA	1795		HIS	244	44.085	16.075		1.00 35.45	Ä
60	MOTA	1796	С	HIS	244	42.108	13.878		1.00 29.05	A
60	MOTA	1797	0	HIS	244	41.541	14.599		1.00 28.16	A
	MOTA	1798	N	MET	245		12.813		1.00 29.99	A
	MOTA	1799	CA	MET	245	42.968	12.425		1.00 32.41	A
	MOTA	1800	CB	MET	245	42.330	11.053		1.00 30.98	A
	ATOM	1801	CG	MET	245	40.880	10.959	116.795	1.00 29.47	A
65	ATOM	1802	SD	MET	245	40.390		116.608	1.00 28.28	A
	ATOM	1803	CE	MET	245	41.018		114.953	1.00 26.37	A
	ATOM	1804	c	MET	245	44.395	12.388		1.00 34.03	A
	ATOM	1805	ŏ	MET	245	45.332	11.978		1.00 33.45.	Ä
	ATOM	1806	N	LYS	246	44.536	12.821		1.00 36.79	Ä
70		1807		LYS	246	45.813	12.821		1.00 36.79	A
, 0	MOTA		CA							
	MOTA	1808	CB	LYS	246	46.345	14.234		1.00 44.53	A
	ATOM	1809	CG	LYS	246	47.765	14.284		1.00 48.98	A
	MOTA	1810	CD	LYS	246	48.360	15.678	120.048	1.00 52.77	A

		1011			246	40.030	15 503		1 00 55 00	
	MOTA	1811	CE	LYS	246	49.830		120.448	1.00 55.09	A
	MOTA	1812	NZ	LYS	246	50.445		120.232	1.00 56.33	A
	ATOM	1813	C	LYS	246	45.496		120.799	1.00 42.14	A
5	MOTA	1814	0	LYS	246	45.157		121.764	1.00 42.94	A
,	MOTA	1815	N	GLU	247	45.586		120.834	1.00 42.88	A
	MOTA	1816	CA	GLU	247	45.286		122.027	1.00 45.27	A A
	MOTA	1817	CB	GLU	247	44.896		121.623	1.00 45.22 1.00 45.70	A
	MOTA	1818	CG	GLU	247	44.301		122.726	1.00 45.70	A
10	MOTA	1819	CD	GLU	247	44.075		122.282	1.00 47.31	A
10	MOTA	1820		GLU	247	43.507		121.186	1.00 47.23	Â
	MOTA MOTA	1821 1822	C	GLU	247 247	44.462 46.463		123.032 122.995	1.00 47.23	Â
	MOTA	1823	ŏ	CLU	247	47.625		122.592	1.00 46.38	A
	MOTA	1824	и	THR	248	46.144		124.281	1.00 47.43	Ä
15	MOTA	1825	CA	THR	248	47.155		125.320	1.00 49.03	Ä
13	ATOM	1826	CB	THR	248	47.340		126.029	1.00 49.86	Ä
	ATOM	1827	0G1		248	47.733		125.066	1.00 50.38	Ä
	MOTA	1828	CG2		248	48.416		127.104	1.00 49.64	λ.
	ATOM	1829	c	THR	248	46.679		126.309	1.00 49.49	A
20	ATOM	1830	ō	THR	248	45.810		127.148	1.00 49.04	Ä
	ATOM	1831	N	THR	249	47.244		126.177	1.00 50-47	A
	MOTA	1832	CA	THR	249	46.892		127.025	1.00 51.50	A
	ATOM	1833	CB	THR	249	47.684		126.621	1.00 51.30	A
	ATOM	1834		THR	249	49.072		126.933	1.00 50.45	A
25	MOTA	1835	CG2		249	47.539		125.127	1.00 50.34	A
	ATOM	1836	С	THR	249	47.157		128.493	1.00 52.76	А
	ATOM	1837	ō	THR	249	47.801		128.819	1.00 52.66	A
	ATOM	1838	N	ILE	250	46.663	5.948	129.375	1.00 53.97	A
	MOTA	1839	CA	ILE	250	46.842	6.136	130.812	1.00 55.19	A
30	MOTA	1840	CB	ILE	250	46.042	5.078	131.624	1.00 55.38	A
	MOTA	1841	CG2	ILE	250	44.596	5.061	131.147	1.00 55.55	A
	MOTA	1842	CG1	ILE	250	46.656	3.683	131.466	1.00 55.59	'A
	MOTA	1843	CD1	ILE	250	46.516	3.078	130.073	1.00 56.12	A
	MOTA	1844	С	ILE	250	48.313	6.097	131.239	1.00 55.82	A
35	MOTA	1845	0	ILE	250	48.634	6.316	132.408	1.00 55.54	A
	MOTA	1846	N	ASP	251	49.198	5.833	130.281	1.00 56.61	A
	MOTA	1847	CA	ASP	251	50.633	5.776	130.543	1.00 57.44	A
	MOTA	1848	CB	ASP	251	51.285	4.696	129.679	1.00 57.92	A
40	MOTA	1849	CG	ASP	251	50.757	3.306	129.979	1.00 58.92	A
40	MOTA	1850	OD1	ASP	251	50.894	2.427	129.098	1.00 59.53	A
	ATOM	1851	OD2	ASP	251	50.217		131.089	1.00 57.67	A
	ATOM	1852	C	ASP	251	51.271		130.222	1.00 57.89	A
	MOTA	1853	0	ASP	251	51.858		131.090	1.00 59.32	A
45	MOTA	1854	N	GLY	252	51.141		128.967	1.00 57.36	A
45	MOTA	1855	CA	GLY	252	51.707		128.526	1.00 57.52	A
	MOTA	1856	С	GLY	252	52.089		127.060	1.00 57.92	A
	MOTA	1857	0	GLY	252	52.814		126.545	1.00 58.43	A
	MOTA	1858	N	GLU	253	51.602		126.392	1.00 57.56	λ
50	MOTA	1859	CA	GLU	253	51.869		124.974	1.00 57.81	A
50	MOTA	1860	CB	GLU	253	51.552		124.598	1.00 59.90	A
	MOTA	1861	CC	GLU	253	52.084		125.573	1.00 62.49	A
	MOTA	1862	CD	GLU	253	51.543		125.294	1.00 63.65	A
	MOTA	1863		GLU	253	51.693		124.146	1.00 65.45	A
55	MOTA	1864		GLU	253	50.970		126.219	1.00 63.15	A
JJ	MOTA	1865	C	GLU	253	50.959		124.179	1.00 56.36	A
	MOTA	1866	0	GLU	253	49.818		124.572	1.00 56.13	A
	ATOM	1867		·GLU	254	51.451		123.067	1.00 54.64	A
	MOTA	1868	CA	GLU	254	50.626		122.256	1.00 53.82 1.00 54.89	A
60	MOTA	1869 1870	CB	GLU	254	51.269		122.151	1.00 56.86	A A
UU	MOTA		CG	GLU	254	52.568	11.259	121.354	1.00 58.42	
	MOTA	1871 1872		GLU	254	52.363		119.939		A
	ATOM			GLU	254	51.856		119.800	1.00 58.67 1.00 57.93	A
	ATOM	1873		GLU -		52.713		118.968	1.00 57.93	A A
65	MOTA MOTA	1874 1875	C	GLU	254	50.397		120.876	1.00 52.35	A
55		1876	0	GLU	254	51.340 49.135		120.124	1.00 50.68	
	ATOM		N	LEU	255				1.00 48.63	A
	MOTA	1877	CA	LEU	255	48.772		119.268	1.00 49.85	A A
	MOTA MOTA	1878 1879	CB	LEU	255 255	47.828 48.236		119.439 120.231	1.00 49.83	A
70	ATOM	1880		LEU	255 255	48.236		119.752	1.00 53.67	A
, 0	ATOM	1881		LEU		48.278		121.720	1.00 53.72	A
	ATOM	1882	C	LEU	255 255	48.278		118.413	1.00 46.05	Â
	MOTA	1883	0	LEU	255	46.978		118.755	1.00 45.38	A
	AT OU	1007	v	250	433	40.315	3.032	110.733	1.00 12.30	

									•	
	MOTA	1884	N	VAL	256	48.695	9:772	117.310	1.00 43.74	· A
	MOTA	1885	CA	VAL	256	48.081		116.409	1.00 41.19	A
	MOTA	1886	CB	VAL	256	49.084		115.943	1.00 40.17	Α
_	ATOM	1887	CG1	VAL	256	48.442	12.680	114.897	1.00 38.91	A
5	MOTA	1888		VAL	256	49.543		117.132	1.00 40.08	A
	MOTA	1889	C	VAL	256	47.533		115.200	1.00 39.59	λ
	MOTA	1890	0	VAL	256	48.276		114.291	1.00 39.95	A
	MOTA	1891	N	LYS	257	46.221		115.212	1.00 36.47	A
10	MOTA MOTA	1892 1893	CA CB	LYS LYS	257 257	45.534		114.150	1.00 32.43	A
10	MOTA	1894	CG	LYS	257	44.733 45.525		114.756 115.710	1.00 31.46	A
	ATOM	1895	CD	LYS	257	44.613		116.573	1.00 31.17 1.00 30.49	A A
	MOTA	1896	CE	LYS	257	43.767		117.486	1.00 30.49	Ã
	MOTA	1897	NZ	LYS	257	42.941		118.411	1.00 32.10	Ä
15	MOTA	1898	C	LYS	257	44.585		113.384	1.00 30.18	A
	MOTA	1899	Ó	LYS	257	44.067		113.928	1.00 28.57	A
	MOTA	1900	N	ILE	258	44.361		112.120	1.00 28.11	A
	MOTA	1901	CA	ILE	258	43.451	10.372	111.263	1.00 26.14	A
20	MOTA	1902	CB	ILE	258	44.223	11.174	110.209	1.00 26.23	A
20	MOTA	1903		ILE	258	43.265		109.205	1.00 26.22	· A
	MOTA	1904		ILE	258	45.027		110.904	1.00 27.27	A
	MOTA	1905		ILE	258	45.828		109.943	1.00 29.18	A.
	MOTA	1906	c	ILE	258	42.493		110.573	1.00 24.09	A
25	HOTA MOTA	1907 1908	O N	ILE GLY	258 259	42.912 41.208		109.772	1.00 24.80	A
LJ	ATOM	1909	CA	GLY	259	40.221		110.899	1.00 20.82 1.00 17.04	A
	MOTA	1910	c	GLY	259	39.214		109.447	1.00 17.04	A A
	MOTA	1911	ŏ	GLY	259	38.843		109.765	1.00 14.10	Ä
	ATOM	1912	N	LYS	260	38.782		108.349	1.00 13.62	A
30	MOTA	1913	CA	LYS	260	37.803		107.487	1.00 13.15	A
	MOTA	1914	CB	LYS	260	38.480		106.247	1.00 13.95	A
	MOTA	1915	CG	LYS	260	37.557	10.866	105.414	1.00 14.12	A
	MOTA	1916	CD	LYS	260	38.254	11.500	104.220	1.00 14.32	A
25	MOTA	1917	CE	LYS	260	37.256		103.410	1.00 16.28	A
35	MOTA	1918	NZ	LYS	260	37.881		102.307	1.00 14.26	A
	MOTA	1919	C	LYS	260	36.687		107.080	1.00 13.76	A
	MOTA MOTA	1920	0	LYS	260	36.939		106.612	1.00 14.46	A
	MOTA	1921 1922	N CA	LEU	261 261	35.449 34.281		107.277	1.00 11.00	A
40	MOTA	1923	CB	LEU	261	33.461	8.067 7.830	106.954	1.00 9.03 1.00 6.67	A
	ATOM	1924	CG	LEU	261	32.123		108.093	1.00 3.68	A A
	MOTA	1925		LEU	261	32.319		107.514	1.00 2.23	A
	MOTA	1926		LEU	261	31.499	7.027		1.00 3.51	A
	MOTA	1927	С	LEU	261	33.416		105.905	1.00 10.81	Α
45	MOTA	1928	0	LEU	261	32.978	9.914	106.113	1.00 9.03	A
	MOTA	1929	N	asn	262	33.180		104.786	1.00 8.62	A
	MOTA	1930	CA	ASN	262	32.360		103.702	1.00 9.89	A
	MOTA	1931	CB	ASN	262	33.042		102.348	1.00 10.45	A
50	ATOM ATOM	1932 1933	CG OD1	ASN ASN	262 262	34.436 35.420		102.294	1.00 14.30	A
-	ATOM	1934	ND2		262	34.535		102.136	1.00 16.96 1.00 9.79	A A
	ATOM	1935	c	ASN	262	31.003	7.905	103.721	1.00 9.32	Ä
	MOTA	1936	ō	ASN	262	30.940		103.638	1.00 10.83	Ä
	MOTA	1937	N	LEU	263	29.923		103.839	1.00 8.87	λ
55	ATOM	1938	CA	LEU	263	28.572	8.108	103.874	1.00 8.66	Α
	MOTA	1939	CB	LEU	263	27.832	8.607	105.108	1.00 6.12	A
	MOTA	1940	CG	LEU	263	28.620	8.253	106.375	1.00 8.11	A
	MOTA	1941	CD1		263	27.981		107.599	1.00 8.26	A
60	MOTA	1942	CD2		263	28.679		106.520	1.00 5.47	A
00	MOTA	1943	C	LEU	263	27.878		102.595	1.00 10.21	A
	ATOM	1944	0	LEU	263	27.488		102.441	1.00 12.04	A
	MOTA MOTA	1945 1946	N CA	VAL: VAL	264 264	27.716		101.682 100.378	1.00 9.38	A
	ATOM	1947	СВ	VAL	264	27.161 28.089	7.329	99.291	1.00 9.77 1.00 10.33	A
65	ATOM	1948	CG1		264	27.734	7.907	97.928	1.00 10.33	A A
	MOTA	1949	CG2		264	29.522	7.637	99.672	1.00 8.80	A
	ATOM	1950	c	VAL	264	25.765		100.104	1.00 10.32	Ä
	ATOM	1951	ō	VAL	264	25.465		100.226	1.00 12.03	Ä
70	MOTA	1952	N	ASP	265	24.925	8.355	99.714	1.00 9.00	A
70	MOTA	1953	CA	ASP	265	23.534	8.116	99.368	1.00 6.24	A
	MOTA	1954	СВ	ASP	265	22.650	9.211	99.985	1.00 5.48	A
	MOTA	1955	CG-	ASP	265	21.171	8.994	99.713	1.00 7.76	A
	MOTA	1956	OD1	ASP	265	20.851	8.232	98.782	1.00 5.27	A

					266	20 222				
	MOTA	1957	OD2		265	20.328		100.421	1.00 9.82	A
	MOTA	1958	С	ASP	265	23.497	8.203	97.838	1.00 4.32	A
	ATOM	1959	0	ASP	265	23.410	9.289	97.270	1.00 4.24	A
_	MOTA	1960	N	LEU	266	23.575	7.060	97.172	1.00 4.44	A
5	MOTA	1961	CA	LEU	266	23.569	7.024	95.710	1.00 5.61	A
	MOTA	1962	CB	LEU	266	23.941	5.616	95.222	1.00 1.02	A
	MOTA	1963	CG	LEU	266	25.345	5.124	95.622	1.00 5.57	A
	MOTA	1964		LEU	266	25.561	3.649	95.242	1.00 1.02	A
	ATOM			LEU	266	26.379	6.020	94.942	1.00 4.62	A
10		1965								
10	MOTA	1966	C	LEU	266	22.252	7.451	95.065	1.00 7.56	A
	MOTA	1967	0	LEU	266	21.190	7.438	95.694	1.00 9.23	A
	MOTA	1968	N	ALA	267	22.336	7.845	93.801	1.00 7.43	A
	MOTA	1969	CA	ALA	267	21.156	8.220	93.047	1.00 6.36	A
	MOTA	1970	CB	ALA	267	21.572	8.756	91.687	1.00 5.05	A
15	ATOM	1971	С	ALA	267	20.324	6.945	92.877	1.00 6.99	A
	MOTA	1972	0	ALA	267	20.844	5.840	93.020	1.00 5.27	A
	MOTA	1973	N	GLY	268	19.042	7.105	92.571	1.00 9.81	A
	MOTA	1974	CA	GLY	-268	18.170	5.961	92.378	1.00 12.51	A
	MOTA	1975	C	GLY	268	18.633	5.079	91.233	1.00 15.67	A
20	ATOM	1976	ŏ	GLY	268	18.859	5.555	90.113	1.00 17.12	A
	ATOM	1977	N	SER	269	18.755	3.786	91.516	1.00 15.31	Ä
	MOTA	1978	CA	SER	269	19.220	2.802	90.543	1.00 18.23	Ä
		1979	CB	SER	269	19.677	1.554	91.293	1.00 17.50	Ä
	MOTA									
25	MOTA	1980	OG	SER	269	18.596	1.027	92.043	1.00 12.64	y
23	MOTA	1981	С	SER	269	18.195	2.383	89.484	1.00 20.29	A
	MOTA	1982	0	SER	269	18.497	1.549	88.627	1.00 19.97	λ
	MOTA	1983	N	GLU	270	16.994	2.950	89.537	1.00 22.91	A
	MOTA	1984	CA	GLU	270	15.949	2.576	88.587	1.00 26.68	A
00	MOTA	1985	CB	GLU	270	14.563	2.958	89.136	1.00 24.65	A
30	MOTA	1986	CG	GLU	270	14.251	4.460	89.210	1.00 22.35	A
	MOTA	1987	CD	GLU	270	14.960	5.185	90.349	1.00 21.47	A
	MOTA	1988	OE1	GLU	270	15.545	4.524	91.234	1.00 18.55	A
	MOTA	1989	OE2	GLU	270 ·	14.922	6.433	90.354	1.00 22.04	A
	MOTA	1990	c	GLU	270	16.117	3.139	87.177	1.00 31.14	A
35	ATOM	1991	ō	GLU	270	16.608	4.256	86.981	1.00 30.32	A
	ATOM	1992	N	ASN	271	15.717	2.336	86.194	1.00 36.67	A
	MOTA	1993	CA	ASN	271	15.799	2.730	84.793	1.00 41.70	A
	MOTA	1994	CB	ASN	271	16.856	1.900	84.059	1.00 45.31	Α
	MOTA	1995	CG	ASN	271	17.121	2.409	82.649	1.00 49.20	A
40	ATOM	1996	OD1		271	17.661	3.504	82.460	1.00 50.16	Ä
70	MOTA	1997	ND2		271	16.733	1.618	81.650	1.00 50.41	À
										A
	MOTA	1998	c	ASN	271	14.440	2.537	84.120	1.00 42.80	
	MOTA	1999	0	ASN	271	13.799	1.494	84.276	1.00 44.21	A
45	ATOM	2000	N	ASN	287	17.192	11.408	81.710	1.00 47.26	A
43	ATOM	2001	CA	ASN	287	18.348	11.168	80.854	1.00 46.49	Α
	MOTA	2002	CB	ASN	287	19.078	12.487	80.582	1.00 48.42	A
	MOTA	2003	CG	ASN	287	18.323	13.385	79.614	1.00 51.20	A
	MOTA	2004		ASN	287	18.724	14.526	79.368	1.00 51.62	A
	MOTA	2005	ND2	ASN	287	17.230	12.870	79.053	1.00 50.69	A
50	MOTA	2006	С	ASN	287	19.324	10.139	81.437	1.00 45.61	A
	MOTA	2007	0	ASN	287	18.912	9.131	82.021	1.00 45.57	A
	MOTA	2008	N	ILE	288	20.619	10.400	81.285	1.00 42.07	A
	MOTA	2009	CA	ILE	288	21.634	9.471	81.771	1.00 37.70	A
	ATOM	2010	CB	ILE	288	22.657	9.156	80.646	1.00 39.37	A
55	MOTA	2011	CG2		288	21.964	.8.416	79.511	1.00 38.36	A
	MOTA	2012	CG1		288	23.269	10.450	80.095	1.00 40.59	A
	MOTA	2013		ILE	288	24.498	10.959	80.863	1.00 42.56	A
	ATOM						9.924	83.019	1.00 33.61	Ä
		2014	C	ILE	288	22.385				λ
60	ATOM	2015	0	ILE	288	22.668	11.113	83.194	1.00 34.30	
w	ATOM	2016	N	ASN	289	22.682	8.970	83.897	1.00 26.00	A
	MOTA	2017	CA	ASN	289	23.431	9.267	85.107	1.00 19.08	A
	MOTA	2018	CB	ASN	289	22.810	8.599	86.334	1.00 17.79	A
	MOTA	2019	CG	asn	289	23.253	9.253	87.645	1.00 18.18	A
/-	MOTA	2020	OD1		289	22.461	9.928	88.299	1.00 18.30	A
65	MOTA	2021	ND2	ASN	289	24.516	9.065	88.023	1.00 13.15	A
	MOTA	2022	С	ASN	289	24.808	8.679	84.861	1.00 15.55	A
	MOTA	2023	ō	ASN	289	25.033	7.493	85.072	1.00 12.50	A
	MOTA	2024	N	GLN	290	25.727	9.515	84.398	1.00 13.86	A
	MOTA	2025	CA	GLN	290	27.079	9.070	84.088	1.00 12.24	A
70	MOTA	2026	CB	GLN	290	27.896	10.253	83.560	1.00 11.18	Ä
		2027	CG	GLN	290	29.284	9.913	83.068	1.00 10.23	Ä
	MOTA			GLN			8.795		1.00 10.23	A
	MOTA	2028	CD		290	29.297		82.036	1.00 11.80	A
	MOTA	2029	OE1	OPN	290	28.336	8.609	81.273	1.00 12.41	~

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	MOTA	2030		GLN	290	30.399	8.059	81.990	1.00 10.69	A
	MOTA	2031	С	GLN	290	27.778	8.414	85.276	1.00 11.63	A
	MOTA	2032	0	GLN	290	28.394	7.359	85.130	1.00 12.20	A
	ATOM	2033	N	SER	291	27.662	9.023	86.452	1.00 10.76	A
5	ATOM	2034	CA	SER	291	28.304	8.485	87.650	1.00 11.04	A
_	MOTA	2035	CB	SER	291	28.163	9.450	88.830	1.00 10.12	A
								88.711	1.00 11.06	A
	ATOM	2036	0G	SER	291	29.068	10.536			
	MOTA	2037	С	SER	291	27.753	7.131	88.043	1.00 11.79	A
	MOTA	2038	0	SER	291	28.512	6.241	88.420	1.00 14.45	A
10	ATOM	2039	N	LEU	292	26.437	6.971	.87.959	1.00 11.86	A
	ATOM	2040	CA	LEU	292	25.805	5.709	88.312	1.00 10.53	A
	MOTA	2041	СВ	LEU	292	24.278	5.875	88.329	1.00 10.11	A
	ATOM	2042	CG	LEU	292	23.467	4.734	88.952	1.00 11.58	A
15	ATOM	2043		LEU	292	23.811	4.605	90.427	1.00 9.76	A
15	MOTA	2044		LEU	292	21.974	5.007	88.791	1.00 11.92	A
	MOTA	2045	С	LEU	292	26.216	4.653	87.289	1.00 10.87	A
	MOTA	2046	0	LEU	292	26.559	3.525	87.634	1.00 12.05	A
	ATOM	2047	N	LEU	293	26.196	5.043	86.022	1.00 11.04	A
	ATOM	2048	CA	LEU	293	26.566	4.165	84.929	1.00 11.19	A
20	ATOM	2049	СВ	LEU	293	26.382	4.922	83.608	1.00 11.77	A
							4.442		1.00 15.36	A
	ATOM	2050	CC.	LEU	293	25.394		82.532		
	ATOM	2051		LEU	293	24.197	3.755	83.162	1.00 13.37	A.
	ATOM	2052	CD2	LEU	293	24.948	5.638	81.690	1.00 11.70	A
	ATOM	2053	С	LEU	293	28.026	3.714	85.094	1.00 13.10	A
25	ATOM	2054	0	LEU	293	28.355	2.535	84.918	1.00 13.28	Α
	MOTA	2055	N	THR	294	28.896	4.660	85.437	1.00 11.21	A
	ATOM	2056	CA	THR	294	30.313	4.372	85.613	1.00 10.86	A
									1.00 12.02	
	MOTA	2057	CB	THR	294	31.119	5.690	85.778		A
20	MOTA	2058	0G1	THR	294	30.934	6.497	84.611	1.00 11.95	Α
30	MOTA	205 9	CG2	THR	294	32.605	5.409	85.947	1.00 8.75	A
	MOTA	2060	С	THR	294	30.571	3.459	86.809	1.00 11.13	A
	ATOM	2061	0	THR	294	31.416	2.563	86.735	1.00 10.49	A
	MOTA	2062	N	LEU	295	29.843	3.686	87.906	1.00 11.70	A
	ATOM	2063	CA	LEU	295	29.983	2.870	89.117	1.00 11.27	A
35	ATOM		CB	LEU	295			90.224	1.00 10.76	Ä
55		.2064				29.033	3.348			
	MOTA	2065	CG	LEU	295	28.993	2.535	91.529	1.00 10.99	A
	MOTA	2066		LEU	295	30.352	2.540	92.214	1.00 12.41	λ
	ATOM	2067	CD2	LEU	295	27.950	3.126	92.458	1.00 10.86	A
	ATOM	2068	С	LEU	295	29.683	1.424	88.788	1.00 10.80	A
40	ATOM	2069	0	LEU	295	30.365	0.521	89.252	1.00 12.59	A
	ATOM	2070	N	GLY	296	28.652	1.205	87.986	1.00 11.95	A
	ATOM	2071	CA	GLY	296	28.311	-0.153	87.607	1.00 12.43	λ
	MOTA	2072	c	GLY	296	29.444	-0.772	86.810	1.00 13.06	A
15	MOTA	2073	0	GLY	296	29.796	-1.938	87.007	1.00 15.18	A
45	MOTA	2074	N	ARG	297	30.021	0.014	85.906	1.00 11.06	A
	MOTA	2075	CA	ARG	297	31.121	-0.458	85.086	1.00 9.97	A
	ATOM	2076	CB	ARG	297	31.369	0.517	83.943	1.00 9.77	A
	ATOM	2077	CG	ARG	297	30.264	0.487	82.909	1.00 10.57	A
	ATOM	2078	CD	ARG	297	30.173	1.789	82.136	1.00 8.79	A
50		2079	NE	ARG		29.014	1.776	81.259	1.00 10.33	A
50	MOTA				297					
	MOTA	2080	CZ	ARG	297	28.492	2.853	80.685	1.00 9.93	A
	MOTA	2081	NH1	ARG	297	29.033	4.044	80.892	1.00 10.65	A
	MOTA	2082	NH2	ARG	297	27.412	2.740	79.920	1.00 7.47	A
	MOTA	2083	С	ARG	297	32.395	-0.675	85.889	1.00 9.24	A
55	MOTA	2084	0	ARG	297	33.154	-1.597	85.594	1.00 10.04	A
	ATOM	2085	N	VAL	298	32.632	0.164	86.897	1.00 6.73	A
	MOTA	2086	CA	VAL	298	33.823	0.009	87.734	1.00 7.78	A
	ATOM	2087	СВ	VAL	298	33.988	1.196	88.719		A
(0	MOTA	2088		VAL	298	35.026	0.865	89.773	1.00 2.16	A
60	ATOM	2089	CG2	VAL	298	34.408	2.449	B7.957	1.00 4.22	A
	ATOM	2090	C	VAL	298	33.775	-1.315	88.517	1.00 9.86	A
	MOTA	2091	0	VAL	298	34.761	-2.057	88.556	1.00 11.69	A
	ATOM	2092	N	ILE	299	32.625	-1.616	89.120	1.00 10.47	A
		2093			299	32.437		89.879	1.00 10.02	
65	MOTA		CA	ILE			-2.858			A
O)	ATOM	2094	CB	ILE	299	31.004	-2.910	90.488	1.00 10.33	A
	MOTA	2095	CG2		299	30.710	-4.280	91.095	1.00 9.07	A
	MOTA	2096		ILE	299	30.869	-1.821	91.558	1.00 10.35	A
	MOTA	2097	CD1	ILE	299	29.445	-1.587	92.019	1.00 13.51	A
	ATOM	2098	С	ILE	299	32.659	-4.070	88.972	1.00 11.19	A
70	MOTA	2099	ō	ILE	299	33.341	-5.019	89.348	1.00 9.09	A
, ,			N				-4.031	87.771	1.00 14.08	A
	MOTA	2100		THR	300	32.084				
	MOTA	2101	CA	THR	300	32.227	-5.125	86.808	1.00 13.98	A
	ATOM	2102	CB	THR	300	31.470	-4.813	85.506	1.00 13.76	A

	MOTA	2103	ogi T	HR 300	30.062	-4.803	85.770	1.00 14.55	A
	MOTA	2104	CG2 T	HR 300	31.783	-5.848	84.436	1.00 10.43	A
	MOTA	2105		HR 300	33.699	-5.394	86.472	1.00 16.17	A
5	ATOM	2106		HR 300	34.151	-6.536	86.533	1.00 16.23	y
5	MOTA	2107		LA 301	34.442	-4.345	86.120	1.00 15.12	A A
	MOTA MOTA	2108 2109		LA 301 LA 301	35.850 36.449	-4.502 -3.157	85.791 85.362	1.00 14.70	A
	MOTA	2110		LA 301	36.622	-5.068	86.985	1.00 14.94	Ä
	MOTA	2111		LA 301	37.512	-5.893	86.819	1.00 15.20	A
10	MOTA	2112		EU 302	36.282	-4.620	88.188	1.00 16.14	A
	MOTA	2113		EU 302	36.951	~5.101	89.392	1.00 19.53	Α
	MOTA	2114		EU 302	36.585	-4.222	90.594	1.00 19.74	A
	ATOM	2115		EU 302	37.221	-2.830	90.688	1.00 17.91	A
15	MOTA	2116	CD1 L		36.558	-2.045	91.802	1.00 17.40	A
13	MOTA	2117	CD2 LI		38.717	-2.963	90.948	1.00 15.50	A A
	MOTA MOTA	2118 2119		EU 302 EU 302	36.643 37.533	-6.564 -7.302	89.717 90.127	1.00 21.83	Ä
	MOTA	2120		AL 303	35.398	-6.993	89.535	1.00 24.49	A
	ATOM	2121		AL 303	35.059	-B.379	89.838	1.00 27.38	A
20	ATOM	2122		AL 303	33.547	-8.571	90.069	1.00 26.90	A
	MOTA	2123	CG1 V	AL 303	33.052	-7.570	91.101	1.00 26.40	A
	MOTA	2124	CG2 V		32.796	-8.428	88.770	1.00 29.98	A
	ATOM	2125		AL 303	35.512	-9.341	88.744	1.00 30.52	A
25	MOTA	2126		AL 303	35.877	-10.477	89.035	1.00 31.69	A
23	MOTA MOTA	2127 2128		LU 304	35.491	-8.897	87.490 86.389	1.00 32.89 1.00 35.74	A A
	MOTA	2128		LU 304 LU 304	35.921 35.203	-9.750 -9.374	85.094	1.00 33.74	A
	MOTA	2130		LU 304	33.689	-9.307	85.221	1.00 39.61	Ä
	ATOM	2131		LU 304	32.999	-9.146	83.876	1.00 42.09	A
30	MOTA	2132	OE1 G		33.515	-8.380	83.028	1.00 42.71	A
	MOTA	2133	OE2 G	LU 304	31.939	-9.775	83.671	1.00 41.78	A
	MOTA	2134		LU 304	37.426	-9.604	86.206	1.00 37.86	A
	ATOM	2135		LU 304	37.996	-10.078	85.227	1.00 37.10	A
35	ATOM	2136		RG 305	38.054	-8.937	87.169 87.177	1.00 40.46 1.00 42.89	A A
23	ATOM ATOM	2137 2138		RG 305	39.496 40.215	-8.716 -10.025	87.534	1.00 42.89	A
	ATOM	2139		RG 305	40.201	-10.328	89.040	1.00 50.55	A
	MOTA	2140		RG 305	40.942	-9.222	89.795	1.00 55.95	A
	ATOM	2141		RG 305	40.641	-9.139	91.227	1.00 60.56	A
40	MOTA	2142	CZ A	RG 305	41.079	-9.988	92.154	1.00 62.46	Α.
	MOTA	2143	NH1 A		41.848	-11.016	91.816	1.00 63.45	A
	MOTA	2144	NH2 AI		40.765	-9.793	93.431	1.00 62.35	A
	MOTA MOTA	2145 2146		RG 305	40.094 41.257	-8.101 -8.337	85.913 85.585	1.00 43.03 1.00 42.44	A A
45	ATOM	2147		RR 306	39.292	-7.300	85.218	1.00 43.37	Ä
	ATOM	2148		HR 306	39.728	-6.607	84.009	1.00 43.89	A A
	MOTA	2149		IR 306	38.553	-5.823	83.373	1.00 44.73	A
	ATOM	2150	OG1 TI	HR 306	37.525	-6.738	82.967	1.00 46.53	A
50	MOTA	2151	CG2 TI	HR 306	39.021	-5.031	82.173	1.00 44.99	A
50	ATOM	2152		R 306	40.816	-5.616	84.428	1.00 43.35	A
	ATOM	2153		R 306	40.648	-4.883	85.405	1.00 44.14	A
	MOTA MOTA	2154 2155		RO 307	- 41.944 42.230	-5.572 -6.282	83.696 82.436	1.00 42.66	A A
	ATOM	2156		RO 307	43.039	-4.651	84.035	1.00 41.12	Ä
55	MOTA	2157		RO 307	44.109	-4.993	83.001	1.00 41.90	A
	MOTA	2158		RO 307	43.302	-5.410	81.811	1.00 42.89	A
	MOTA	2159	C PI	RO 307	42.661	-3.165	84.023	1.00 39.78	A
	MOTA	2160		RO 307	43.151	-2.384	84.847	1.00 38.90	A
6 0	MOTA	2161		rs 308	41.789	-2.773	83.099	1.00 36.76	A
60	MOTA	2162	CA H		41.373	-1.381	83.018	1.00 34.24	A
	MOTA	2163	CB H		41.248	-0.946	81.558	1.00 35.68	A
	MOTA	2164 2165	CD2 H	IS 308	40.936 39.847	0.507	81.395 80.888	1.00 38.11 1.00 39.53	A
	MOTA MOTA	2166	ND1 H		41.794	1.134 1.503	81.809	1.00 39.33	A A
65	MOTA	2167	CE1 H		41.249	2.682	81.565	1.00 39.88	Ä
	MOTA	2168	NE2 H		40.067	2.486	81.006	1.00 40.19	Ä
	ATOM	2169		s 308	40.052	-1.120	83.737	1.00 31.65	A
	ATOM	2170	О Н	rs 308	39.009	-1.661	83.362	1.00 32.49	A
70	ATOM	2171		AL 309	40.117	-0.282	84.769	1.00 26.89	A
70	ATOM	2172		AL 309	38.959	0.101	85.580	1.00 22.85	A
	MOTA	2173		AL 309	39.298	-0.013	87.083	1.00 22.36	A
	MOTA MOTA	2174 2175	CG1 V		38.091 39.765	0.351 -1.427	87.922 87.403	1.00 22.91	A A
	VION	41/3	CGZ VI	-D 309	33.105	-1.42/	07.403	1.00 22.12	A

	MOTA	2176	С	VAL	309	38.629	1.558	85.231	1.00 20.44	A
	ATOM	2177	0	VAL	309	39.450	2.446	85.433	1.00 19.97	A
	ATOM	2178	N	PRO	310	37.421	1.822	84.704	1.00 17.91	A
	ATOM	2179	CD	PRO	310	36.413	0.834	84.277	1.00 14.72	A
5	ATOM	2180	CA	PRO	310	37.019	3.186	84.322	1.00 17.34	A
,										
	MOTA	2181	CB	PRO	310	35.839	2.937	83.386	1.00 15.77	A
	ATOM	2182	CC	PRO	310	35.214	1.699	83.978	1.00 15.26	A
	MOTA	2183	С	PRO	310	36.689	4.227	85.404	1.00 16.65	Α
	ATOM	2184	0	PRO	310	35.673	4.908	85.317	1.00 15.99	A
10	MOTA	2185	N	TYR	311	37.557	4.368	86.402	1.00 18.31	A
	ATOM	2186	CA	TYR	311	37.346	5.335	87.485	1.00 18.33	A
	ATOM	2187	CB	TYR				88.430	1.00 18.13	Ä
					311	38.549	5.374			
	MOTA	2188	CC	TYR	311	38.826	4.115	89.209	1.00 20.50	A
	MOTA	2189		TYR	311	37.943	3.660	90.194	1.00 19.61	A
15	MOTA	2190	CE1	TYR	311	38.242	2.538	90.957	1.00 19.17	A
	MOTA	2191	CD2	TYR	311	40.008	3.407	89.005	1.00 19.30	A
	MOTA	2192	CE2	TYR	311	40.314	2.290	89.759	1.00 18.88	A
	ATOM	2193	CZ	TYR	311	39.432	1.860	90.732	1.00 20.10	A
	HOTA	2194	он	TYR	311	39.754	0.749	91.480	1.00 23.13	A
20										Ä
20	MOTA	2195	C	TYR	311	37.150	6.753	86.969	1.00 19.65	
	MOTA	2196	0	TYR	311	36.288	7.485	87.449	1.00 20.71	A
	ATOM	2197	N	ARG	312	37.967	7.140	85.995	1.00 19.46	Α.
	MOTA	- 2198	CA	ARG	312	37.919	8.484	85.447	1.00 19.67	A
	MOTA	2199	CB	ARG	312	39.223	8.775	84.699	1.00 24.48	· A
25	MOTA	2200	CG	ARG	312	40.470	8.521	85.534	1.00 31.49	A
	MOTA	2201	CD	ARG	312	41.737	8.793	84.742	1.00 38.21	A
	ATOM	2202	NE	ARG	312	41.948	10.223	84.543	1.00 41.59	A
	MOTA	2203	CZ	ARG	312	42.419	11.040	85.479	1.00 43.45	A
20	ATOM	2204	-	ARG	312	42.733	10.564	86.678	1.00 43.96	A
30	ATOM	2205	NH2	ARG	312	42.570	12.332	85.217	1.00 44.26	A
	MOTA	2206	С	ARG	312	36.736	8.826	84.547	1.00 17.18	A
	MOTA	2207	0	ARG	312	36.610	9.976	84.121	1.00 17.17	A
	MOTA	2208	N	GLU	313	35.856	7.869	84.262	1.00 14.11	A
	ATOM	2209	CA	GLU	313	34.729	8.178	83.378	1.00 11.27	A
35	ATOM	. 2210		GLU						
22			CB		313	34.258	6.911	82.646	1.00 10.67	A
	MOTA	2211	CG	GLU	313	35.399	6.213	81.891	1.00 15.89	A
	MOTA	2212	CD	GLU	313	34.946	5.089	80.956	1.00 19.42	A
	ATOM	2213	OE1	GLU	313	35.821	4.301	80.519	1.00 20.64	A
	MOTA	2214	OE2	GLU	313	33.739	4.992	80.641	1.00 19.87	A
40	MOTA	2215	С	GLU	313	33.554	8.893	84.048	1.00 9.14	A
. •	MOTA	2216	ō	GLU	313	32.550	9.155	83.410	1.00 8.08	A
	MOTA	2217	N	SER	314	33.692	9.226	85.327	1.00 9.25	A
	MOTA	2218	CA	SER	314	32.647	9.951	86.051	1.00 11.62	A
4.5	MOTA	2219	CB	SER	314	31.508	9.011	86.467	1.00 14.09	A
45	ATOM	2220	OG	SER	314	31.812	8.354	87.688	1.00 14.04	A
	MOTA	2221	С	SER	314	33.233	10.604	87.298	1.00 11.57	A
	MOTA	2222	0	SER	314	34.283	10.186	87.791	1.00 12.89	A
	MOTA	2223	N	LYS	315	32.541	11.615	87.812	1.00 12.14	A
	MOTA	2224	CA	LYS	315	32.981	12.340	89.002	1.00 14.40	λ
50	ATOM	-2225	CB	LYS	315	32.082	13.556	89.246	1.00 17.33	A
50										
	ATOM	2226	CG	LYS	315	32.015	14.559	88.105	1.00 19.52	A
	MOTA	2227	CD	LYS	315 .	33.175	15.536	88.143	1.00 22.04	A
	MOTA	2228	CE	LYS	315	33.021	16.584	87.054	1.00 22.29	A
	MOTA	2229	NZ	LYS	315	32.991	15.922	85.724	1.00 25.05	A
55	MOTA	2230	С	LYS	315	32.952	11.461	90.253	1.00 14.36	A
	ATOM	2231	0	LYS	315	33.899	11.459	91.042	1.00 15.78	A
	MOTA	2232	N	LEU	316	31.859	10.723	90.430	1.00 12.10	A
		2233	CA	LEU						A
	ATOM				316	31.693	9.864	91.591	1.00 12.11	
<i>6</i> 0	MOTA	2234	CB	LEU	316	30.346	9.132	91.521	1.00 11.47	A
60	ATOM	2235	CC	LEU	316	30.052	8.165	92.673	1.00 11.12	A
	MOTA	2236	CD1	LEU	316	29.755	8.941	93.947	1.00 10.52	A
	ATOM	2237	CD2	LEU	316	28.867	7.294	92.313	1.00 9.92	A
	MOTA	2238	C	LEU	316	32.816	8.846	91.790	1.00 12.47	A
	ATOM	2239	ŏ	LEU	316	33.346	8.720	92.892	1.00 13.63	Ä
65										
U	MOTA	2240	И	THR	317	33.192	8.124	90.738	1.00 13.16	Α
	MOTA	2241	CA	THR	317	34.245	7.118	90.875	1.00 12.10	A
	MOTA	2242	CB	THR	317	34.132	6.031	89.783	1.00 9.66	A
	MOTA	2243	OG1	THR	317	34.077	6.642	88.496	1.00 9.89	Α
	ATOM	2244	CG2		317	32.870	5.200	89.994	1.00 10.70	A
70	ATOM	2245	c	THR	317	35.674	7.681	90.923	1.00 12.84	Ä
. •	MOTA	2246	ò	THR		36.611	6.965	91.270	1.00 13.25	Ä
					317					
	MOTA	2247	N	ARG	318	35.852	8.951	90.575	1.00 13.06	A
	ATOM	2248	CA	ARG	318	37.180	9.544	90.682	1.00 14.05	A

	MOTA	2249	CB	ARG	318	37.326	10.780	89.796	1.00 15.43	A
	MOTA	2250	CG	ARG	318	37.417	10.473	88.319	1.00 20.15	A
	MOTA	2251	CD	ARG	318	37.526	11.755	87.527	1.00 22.93	A
_	ATOM	2252	NE	ARG	318	38.747	12.468	87.865	1.00 27.97	A
5	ATOM	2253	CZ	ARG	318	39.015	13.710	87.482	1.00 32.10	A
	ATOM	2254		ARG	318	38.138	14.383	86.747	1.00 32.47	A
			NH2				14.276		1.00 33.23	
	MOTA	2255			318	40.162		87.833		A
	MOTA	2256	С	ARG	318	37.281	9.948	92.138	1.00 13.35	A
	MOTA	2257	0	ARG	318	38.276	9.679	92.801	1.00 15.31	A
10	MOTA	2258	N	ILE	319	36.222	10.575	92.640	1.00 12.79	A
	MOTA	2259	CA	ILE	319	36.175	11.012	94.030	1.00 11.02	A
	MOTA	2260	CB	ILE	319				1.00 9.24	
						34.837	11.727	94.322		A
	MOTA	2261		ILE	319	34.660	11.958	95.819	1.00 4.84	A
1.5	MOTA	2262	CG1	ILE	319	34.786	13.047	93.561	1.00 9.26	A
15	ATOM	2263	CD1	ILE	319	33.431	13.786	93.692	1.00 9.14	A
	MOTA	2264	С	ILE	319	36.344	9.833	95.002	1.00 12.21	A
	MOTA	2265	ō	ILE	319	37.127	9.913	95.950	1.00 12.33	A
	ATOM	2266	N		320	35.627	8.739	94.752	1.00 10.74	A
				LEU					-	
20	ATOM	2267	CA	LEU	320	35.674	7.577	95.638	1.00 11.28	A
20	MOTA	2268	CB	LEU	320	34.240	7.142	95.965	1.00 8.50	A
	MOTA	2269	CG	LEU	320	33.364	8.196	96.642	1.00 11.65	A
	MOTA	2270	CD1	LEU	320	31.909	7.774	96.550	1.00 12.32	A
	ATOM	2271		LEU	320	33.794	8.390	98.090	1.00 7.79	A
	ATOM	2272								
25			C	LEU	320	36.466	6.359	95.146	1.00 12.31	A
25	MOTA	2273	0	LEU	320	36.276	5.254	95.658	1.00 10.52	A
	MOTA	2274	N	GLN	321	37.356	6.541	94.177	1.00 13.27	A
	MOTA	2275	CA	GLN	321	38.110	5.401	93.668	1.00 16.08	A
	ATOM	2276	CB	GLN	321	39.087	5.844	92.569	1.00 19.75	A
	ATOM	2277	CG	GLN	321	40.196	6.756	93.006	1.00 21.68	A
30		2278							1.00 25.85	
50	MOTA		CD	GLN	321	41.079	7.139	91.840		A
	MOTA	2279		GLN	321	41.622	6.266	91.152	1.00 22.98	A
	MOTA	2280	NE2	GLN	321	41.228	8.450	91.602	1.00 26.88	Α
	ATOM	2281	С	GLN	321	38.842	4.548	94.723	1.00 14.28	A
	MOTA	2282	0	GLN	321	38.972	3.335	94.543	1.00 12.19	A
35	ATOM	2283	N	ASP	322	39.305	5.151	95.817	1.00 12.59	A
	MOTA	2284	CA	ASP	322	39.978	4.351	96.835	1.00 14.78	Ä
	MOTA	2285	CB	ASP	322	40.769	5.230	97.811	1.00 17.14	A
	ATOM	2286	CC	ASP	322	41.787	4.426	98.620	1.00 18.36	A
40	ATOM	2287	OD1	ASP	322	42.588	3.692	98.003	1.00 19.34	A
40	ATOM	2288	OD2	ASP	322	41.791	4.521	99.865	1.00 19.68	A
	ATOM	2289	С	ASP	322	38.988	3.473	97.609	1.00 15.66	A
	MOTA	2290	0	ASP	322	39.384	2.598	98.384	1.00 17.16	A
	ATOM	2291	N	SER	323	37.697	3.696	97.386	1.00 16.21	A
		2292								
45	MOTA		CA	SER	323	36.657	2.915	98.047	1.00 16.47	A
43	MOTA	2293	CB	SER	323	35.436	3.795	98.343	1.00 13.71	A
	MOTA	2294	OG	SER	323	35.749	4.804	99.284	1.00 11.67	A
	MOTA	2295	С	SER	323	36.247	1.735	97.166	1.00 18.02	A
	ATOM	2296	0	SER	323	35.459	0.876	97.574	1.00 18.75	A
	ATOM	2297	N	LEU	324	36.795	1.696	95.956	1.00 18.69	A
50	ATOM	2298	CA	LEU	324	36.495	0.635	95.009	1.00 19.76	Ä
	ATOM	2299	CB	LEU	324		1.225	93.789	1.00 19.37	
						35.782				A
	MOTA	2300	CG	LEU	324	34.461	1.920	94.127	1.00 19.69	A
	MOTA	2301	CD1	LEU	324	34.028	2.781	92.973	1.00 22.50	Α
	ATOM	2302	CD2	LEU	324	33.394	0.887	94.449	1.00 20.33	A
55	ATOM	2303	С	LEU	324	37.789	-0.045	94.591	1.00 21.46	A
	ATOM	2304	0	LEU	324	38.427	0.353	93.618	1.00 23.00	A
	ATOM	2305	N	GLY	325	38.174	-1.074	95.341	1.00 22.77	A
		2306								
	MOTA		CA	GLY	325	39.398	-1.794	95.047	1.00 21.76	A
60	MOTA	2307	C	GLY	325	40.620	-1.028	95.516	1.00 24.37	A
60	MOTA	2308	0	GLY	325	41.718	-1.239	95.005	1.00 24.93	A
	MOTA	2309	N	GLY	326	40.428	-0.132	96.484	1.00 24.40	A
	MOTA	2310	CA	GLY	326	41.526	0.663	97.002	1.00 24.15	A
	ATOM	2311	c	GLY	326	41.897	0.284	98.424	1.00 26.42	Α
65	MOTA	2312	0	GLY	326	41.656	-0.840	98.856	1.00 25.60	A
O)	MOTA	2313	N	ARG	327	42.470	1.220	99.168	1.00 25.86	A
	ATOM	2314	CA	ARG	327	42.875	0.919	100.528	1.00 28.96	A
	ATOM	2315	CB	ARG	327	44.219	1.593	100.834	1.00 32.07	A
	ATOM	2316	CG	ARG	327	45.329	1.220	99.853	1.00 37.14	A
	MOTA	2317	CD	ARG	327	46.714		100.432	1.00 42.74	Ä
70										
, 0	ATOM	2318	NE	ARG	327	47.800	1.031	99.556	1.00 47.24	A
	MOTA	2319	CZ	ARG	327	48.286	1.730	98.530	1.00 49.78	A
	ATOM	2320	NH1		327	47.787	2.926	98.237	1.00 50.77	A
	MOTA	2321	NH2	ARG	327	49.286	1.245	97.805	1.00 49.64	λ

	MOTA	2322	С	ARG	327	41.831	1.320	101.569	1.00 28.96	A
	ATOM	2323	ō	ARG	327	42.157		102.731	1.00 28.88	A
	ATOM	2324	N	THR	328	40.573		101.151	1.00 27.38	À
								102.064		
5	MOTA	2325	CA	THR	328	39.499	_		1.00 23.77	A
ر	ATOM	2326	CB	THR	328	38.678		101.488	1.00 24.66	A
	MOTA	2327	OG1	THR	328	39.529		101.344	1.00 25.37	A
	MOTA	2328	CG2	THR	328	37.510	3.292	102.409	1.00 23.54	A
	ATOM	2329	С	THR	328	38.556	0.611	102.353	1.00 20.49	A
	ATOM	2330	0	THR	328	38.287	-0.213	101.480	1.00 19.13	A
10	MOTA	2331	N	ARG	329	38.072		103.588	1.00 17.06	A
	ATOM	2332	CA	ARG	329	37.139		103.954	1.00 15.33	A
	ATOM	2333	CB	ARG	329	37.126		105.465	1.00 14.79	Ä
	ATOM	2334	CG	ARG	329	36.035		105.878	1.00 15.14	A
15	MOTA	2335	CD	ARG	329	35.989		107.370	1.00 17.09	A
15	MOTA	2336	NE	ARG	329	34.897	-2.947	107.655	1.00 21.72	A
	ATOM	2337	CZ	ARG	329	34.688	-3.553	108.819	1.00 22.49	A
	MOTA	2338	NH1	ARG	329	35.504	-3.343	109.841	1.00 20.08	A
	MOTA	2339	NH2	ARG	329	33.646	-4.366	108.958	1.00 22.92	A
	ATOM	2340	С	ARG	329	35.783	-0.001	103.539	1.00 14.65	A
20	ATOM	2341	0	ARG	329	35.352		104.030	1.00 15.12	A
	ATOM	2342	N	THR	330	35.107		102.640	1.00 12.06	A
	ATOM	2343	CA	THR	330	33.809		102.224	1.00 14.04	A.
	ATOM	2344	CB	THR	330	33.837		100.782	1.00 15.17	Ä.
	ATOM	2345			330					
25				THR		33.694	-0.735	99.847	1.00 18.22	·A
23	MOTA	2346		THR	330	35.147		100.513	1.00 14.36	A
	MOTA	2347	C	THR	330	32.707		102.323	1.00 13.65	A
	MOTA	2348	0	THR	330	32.936	-2.459	102.140	1.00 13.67	A
	MOTA	2349	N	SER	331	31.509	-0.786	102.637	1.00 12.70	A
	MOTA	2350	CA	SER	331	30.340	-1.627	102.740	1.00 10.49	A
30	ATOM	2351	CB	SER	331	29.830	-1.648	104.177	1.00 12.02	A
	ATOM	2352	OG	SER	331	30.860	-2.026	105.072	1.00 18.36	A
	MOTA	2353	С	SER	331	29.259		101.830	1.00 10.83	A
	MOTA	2354	ō	SER	331	29.235		101.555	1.00 B.62	A
	ATOM	2355	N	ILE	332	28.376		101.349	1.00 9.52	A
35.	MOTA	-2356	CA	ILE	332	27.288		100.511	1.00 9.50	
33		2357								A
	ATOM .		CB	ILE	332	27.374	-2.038	99.089	1.00 10.70	A
	MOTA	2358		ILE	332	26.143	-1.622	98.287	1.00 8.05	A
	MOTA	2359		ILE	332	28.650	-1.560	98.394	1.00 9.17	A
40	MOTA	2360	CD1	ILE	332	28.773	-2.094	96.975	1.00 5.23	A
40	ATOM	2361	С	ILE	332	25.993	-1.939	101.138	1.00 9.51	A
	ATOM	2362	0	ILE	332	25.843	-3.127	101.413	1.00 9.19	Α
	MOTA	2363	N	ILE	333	25.074	~1.015	101.391	1.00 9.81	A
	ATOM	2364	CA	ILE	333	23.773	-1.376	101.942	1.00 8.92	A
	ATOM	2365	CB	ILE	333	23.335		103.103	1.00 8.82	A
45	ATOM	2366		ILE	333	21.967		103.614	1.00 7.93	A
	ATOM	2367		ILE	333	24.316		104.272	1.00 6.76	Ä
	ATOM	2368	CD1		333	24.028		105.387	1.00 2.97	A
		2369								
	MOTA		C	ILE	333	22.777		100.797	1.00 9.34	A
50	MOTA	2370	0	ILE	333	22.483	-0.132	100.347	1.00 6.58	A
50	ATOM	2371	N	ALA	334	22.294	-2.376	100.303	1.00 9.13	A
	MOTA	2372	CA	ALA	334	21.325	-2.370	99.215	1.00 8.43	A
	MOTA	2373	CB	ALA	334	21.543	-3.582	98.318	1.00 6.36	A
	MOTA	2374	C	ALA	334	19.903	-2.381	99.807	1.00 8.65	A
	MOTA	2375	0	ALA	334	19.555	-3.232	100.634	1.00 6.98	A
55	MOTA	2376	N	THR	335	19.089	-1.419	99.398	1.00 8.61	A
	MOTA	2377	. CA	THR	335	17.727	-1.334	99.899	1.00 8.77	A
	ATOM	2378	CB	THR	335	17.375	0.092	100.290	1.00 7.57	A
	ATOM	2379	OG1		335	17.538	0.949	99.157	1.00 8.21	A
	MOTA	2380		THR	335	18.276	0.552	101.398	1.00 7.82	A
60										
oo	MOTA	2381	С	THR	335	16.729	-1.820	98.863	1.00 8.70	A
	MOTA	2382	0	THR	335	16.855	-1.530	97.671	1.00 8.21	A
	MOTA	2383	N	ILE	336	15.735	-2.560	99.338	1.00 8.74	A
	ATOM	2384	CA	ILE	336	14.717	-3.124	98.469	1.00 10.87	A
	MOTA	2385	CB	ILE	336	14.998	-4.613	98.216	1.00 10.46	A
65	MOTA	2386	CG2	ILE	336	16.353	-4.769	97.532	1.00 8.62	A
	MOTA	2387		ILE	336	14.943	-5.379	99.543	1.00 10.60	A
	MOTA	2388		ILE	336	14.993	-6.921	99.386	1.00 10.91	A
	MOTA	2389	C	ILE	336	13.291	-2.995	99.004	1.00 12.03	Ä
	ATOM	2390	ō	ILE	336	13.069		100.204	1.00 12.49	Ä
70		2391					-3.056			
	MOTA		N	SER	337	12.331		98.089	1.00 13.93	A
	MOTA	2392	CA	SER	337	10.918	-2.969	98.426	1.00 13.83	A
	ATOM	2393	CB	SER	337	10.180	-2.154	97.359	1.00 14.05	A
	MOTA	2394	OG	SER	337	8.790	-2.436	97.350	1.00 13.32	A

			_							
	MOTA	2395	С	SER	337	10.371	-4.386	98.464	1.00 14.60	A
	ATOM	2396	0	SER	337	10.829	-5.250	97.717	1.00 14.95	A
	MOTA	2397	N	PRO	338	9.398	-4.652	99.350	1.00 15.93	A
	ATOM	2398	CD	PRO	338	8.967		100.483	1.00 16.39	A
5	ATOM	2399	CA	PRO	338	8.809	-5.990	99.451	1.00 15.42	A
,										
	MOTA	2400	CB	PRO	338	8.461		100.921	1.00 15.52	A
	MOTA	2401	CG	PRO	338	7.930		101.176	1.00 17.59	A
	MOTA	2402	С	PRO	338	7.564	-6.138	98.576	1.00 15.52	A
	MOTA	2403	0	PRO	338	6.929	-7.185	98.571	1.00 17.10	A
10	ATOM	2404	N	ALA	339	7.212	-5.091	97.841	1.00 15.73	A
	ATOM	2405	CA	ALA	339	6.023	-5.122	96.989	1.00 17.08	A
	MOTA	2406	CB	ALA	339	5.494	-3.699	96.765	1.00 13.90	A
	MOTA	2407	С	ALA	339	6.255	-5.793	95.647	1.00 17.79	A
	MOTA	2408	0	ALA	339	7.290	-5.586	95.010	1.00 18.27	A
15	MOTA	2409	N	SER	340	5.270	-6.575	95.210	1.00 19.26	A
	ATOM	2410	CA	SER	340	5.339	-7.280	93.933	1.00 20.19	A
	ATOM	2411	CB	SER	340	4.088	-8.151	93.741	1.00 21.56	A
			OG	SER	340	2.909	-7.370	93.812	1.00 24.50	A
	ATOM	2412								
20	MOTA	2413	С	SER	340	5.495	-6.340	92.736	1.00 18.83	A
20	MOTA	2414	0	SER	340	5.977	-6.755	91.687	1.00 17.98	A
	MOTA	2415	N	LEU	341	5.083	-5.084	92.883	1.00 19.49	A
	MOTA	2416	CA	LEU	341	5.212	-4.114	91.793	1.00 21.42	A
	MOTA	2417	CB	LEU	341	4.539	-2.787	92.159	1.00 24.24	A
	MOTA	2418	CG	LEU	341	3.056	-2.763	92.528	1.00 30.57	A
25	MOTA	2419		LEU	341	2.838	-3.310	93.952	1.00 30.86	Ä
25										
	MOTA	2420		LEU	341	2.563	-1.325	92.435	1.00 32.23	A
	MOTA	2421	С	LEU	341	6.678	-3.821	91.452	1.00 20.58	A
	MOTA	2422	0	LEU	341	7.017	-3.528	90.308	1.00 20.62	A
	MOTA	2423	N	ASN	342	7.544	-3.905	92.455	1.00 19.46	A
30	MOTA	2424	CA	ASN	342	8.958	-3.620	92.267	1.00 18.47	A
	ATOM	2425	CB	ASN	342	9.471	-2.863	93.485	1.00 17.34	A
	MOTA	2426	CG	ASN	342	8.662	-1.618	93.763	1.00 16.86	A
	MOTA	2427		ASN	342	8.564	-0.730	92.916	1.00 18.67	A
25	MOTA	2428		ASN	342	8.070	-1.546	94.944	1.00 15.28	A
35	ATOM	2429	С	ASN	342	9.795	-4.871	92.041	1.00 18.85	A
	ATOM	2430	0	ASN	342	10.988	-4.893	92.351	1.00 17.91	A
	MOTA	2431	N	LEU	343	9.170	-5.908	91.493	1.00 17.20	A
	ATOM	2432	CA	LEU	343	9.863	-7.163	91.252	1.00 17.19	A
	ATOM	2433	CB	LEU	343	8.917	-8.179	90.596	1.00 13.78	A
40										
40	MOTA	2434	CG	LEU	343	9.593	-9.472	90.107	1.00 14.61	A
	MOTA	2435		LEU	343		-10.143	91.269	1.00 10.55	A
	MOTA	2436	CD2	LEU	343	8.554	-10.415	89.499	1.00 13.10	A
	MOTA	2437	С	LEU	343	11.115	-7.020	90.399	1.00 17.48	A
	MOTA	2438	0	LEU	343	12.211	-7.377	90.829	1.00 17.34	A
45	MOTA	2439	N	GLU	344	10.946	-6.514	89.184	1.00 19.72	A
	ATOM	2440	CA	GLU	344	12.063	-6.358	88.263	1.00 20.96	A
		2441	CB	GLU		11.598	-5.684	86.969	1.00 24.20	A
	MOTA				344					
	MOTA	2442	CG	GLU	344	12.675	-5.635	85.887	1.00 32.62	A
50	ATOM	2443	CD	GLU	344	12.213	-4.959	84.599	1.00 38.13	A
50	MOTA	2444	OEl	GLU	344	12.908	-5.115	83.566	1.00 40.01	A
	MOTA	2445	OE2	GLU	344	11.165	-4.270	84.617	1.00 41.47	Α
	MOTA	2446	С	GLU	344	13.208	-5.561	88.883	1.00 20.19	A
	ATOM	2447	0	GLU	344	14.371	-5.957	88.791	1.00 20.32	A
	ATOM	2448	N	GLU	345	12.883	-4.441	89.518	1.00 17.74	A
55										
JJ	MOTA	2449	CA	GLU	345	13.909	-3.615	90.130	1.00 18.84	. У
	MOTA	2450	CB	GLU	345	13.335	-2.240	90.496	1.00 21.25	· А
	ATOM	2451	CG	GLU	345	13.076	-1.356	89.281	1.00 24.52	A
	MOTA	2452	CD	GLU	345	14.348	-1.036	88.492	1.00 27.03	A
	MOTA	2453	OE1	GLU	345	14.232	-0.592	87.325	1.00 29.83	A
60	ATOM	2454		GLU	345	15.462	-1.216	89.036	1.00 27.61	A
••	ATOM	2455	C		345		-4.270			Ä
			_					,		
	MOTA	2456	0	GLU	345	15.762	-4.143	91.554	1.00 17.33	λ
	MOTA	2457	N	THR	346	13.760	-4.978	92.140	1.00 14.42	A
	MOTA	2458	CA	THR	346	14.286	-5.649	93.316	1.00 14.40	A
65	MOTA	2459	CB	THR	346	13.160	-6.304	94.138	1.00 15.55	A
-	ATOM	2460		THR	346	12.399	-5.285	94.801	1.00 13.04	A
	ATOM	2461		THR	346	13.735	-7.255	95.171	1.00 15.14	A
	MOTA	2462	C	THR	346	15.302	-6.705	92.896	1.00 14.50	A
70	MOTA	2463	0	THR	346	16.294	-6.922	93.590	1.00 13.63	A
70	MOTA	2464	N	LEU	347	15.061	-7.362	91.763	1.00 14.51	A
	MOTA	2465	CA	LEU	347	16.005	-8.357	91.269	1.00 15.49	A
	ATOM	2466	CB	LEU	347	15.369	-9.222	90.167	1.00 15.24	A
	ATOM	2467	CG	LEU	347		-10.158	90.571	1.00 15.51	A
		2.01		~~0	54.					••

	MOTA	2468	CD1	LEU	347	13.712	-10.902	89.351	1.00 11.90	A
	ATOM	2469	CD2	LEU	347	14.687	-11.142	91.627	1.00 13.17	A
									1.00 16.52	A
	MOTA	2470	С	LEU	347	17.267	-7.666	90.734		
_	ATOM	2471	0	LEU	347	18.376	-8.175	90.908	1.00 18.79	A
5	ATOM	2472	N	SER	348	17.111	-6.513	90.088	1.00 15.74	A
-									1.00 16.97	A
	MOTA	2473	CA	SER	348	18.274	-5.795	89.567		
	MOTA	2474	CB	SER	348	17.857	-4.502	88.872	1.00 17.03	A
	MOTA	2475	OG	SER	348	17.008	-4.785	87.780	1.00 23.78	A
10	MOTA	2476	С	SER	348	19.199	-5.438	90.712	1.00 16.29	A
10	ATOM	2477	0	SER	348	20.415	-5.668	90.655	1.00 17.03	A
					349				1.00 13.43	A
	MOTA	2478	N	THR		18.603	-4.864	91.751		
	MOTA	2479	CA	THR	349	19.341	-4.452	92.925	1.00 12.53	A
	MOTA	2480	CB	THR	349	18.400	-3.808	93.953	1.00 11.53	A
1.5	ATOM	2481		THR	349	17.883	-2.583	93.416	1.00 12.14	A
15	MOTA	2482	CG2	THR	349	19.143	-3.512	95.243	1.00 8.21	A
	MOTA	2483	С	THR	349	20.074	-5.624	93.563	1.00 12.73	A
	ATOM	2484	0	THR	349	21.292	-5.590	93.732	1.00 10.74	A
	ATOM	2485	N	LEU	350	19.325	-6.660	93.916	1.00 14.33	A
	MOTA	2486	CA	LEU	350	19.923	-7.830	94.532	1.00 16.65	A
20										
20	ATOM	2487	CB	LEU	350	18.855	-8.892	94.803	1.00 14.51	A
	ATOM	2488	CG	LEU	350	17.916	-8.537	95.960	1.00 13.75	A
	MOTA	2489		LEU	350	16.780	-9.516	96.035	1.00 10.80	A
	ATOM	2490	CD2	LEU	350	18.703	-8.526	97.258	1.00 15.25	A
	ATOM	2491	С	LEU	350	21.033	-8.400	93.660	1.00 17.62	- A
25										
25	MOTA	2492	0	LEU	350	22.116	-8.695	94.148	1.00 19.69	A
	MOTA	2493	N	GLU	351	20.774	-8.540	92.368	1.00 18.77	A
	MOTA	2494	CA	GLU	351	21.783	-9.078	91.466	1.00 20.26	A
	MOTA	2495	CB	GLU	351	21:203	-9.215	90.061	1.00 23.16	A
	ATOM	2496	CG	GLU	351	21.961	-10.194	89.186	1.00 31.07	A
30	MOTA	2497	CD	GLU	351		-11.652	89.508	1.00 35.15	A
50										
	MOTA	2498	OEI	GLU	351	22,421	-12.531	89.070	1.00 37.94	A
	ATOM	2499	OE2	GLU	351	20.621	-11.921	90.180	1.00 35.11	Α
		2500						91.440	1.00 18.73	A
	MOTA		С	GLU	351	23.030	-8.181	-		
	MOTA	2501	0	GLU	351	24.163	-8.662	91.407	1.00 18.86	A
35	MOTA	.2502	N	TYR	352	22.810	-6.873	91.463	1.00 18.82	A
	MOTA	2503	CA	TYR	352	23.893	-5.898	91.443	1.00 16.90	A
	MOTA	2504	CB	TYR	352	23.304	-4.500	91.261	1.00 17.28	A
	MOTA	2505	CG	TYR	352	24.306	-3.374	91.118	1.00 15.30	A
40	MOTA	2506	CDI	TYR	352	24.940	-2.833	92.227	1.00 12.89	A
40	ATOM	2507	CEl	TYR	352	25.779	-1.740	92.100	1.00 15.82	Α
	ATOM	2508		TYR	352	24.550	-2.798	89.869	1.00 15.34	A
	ATOM	2509	CE2	TYR	352	25.382	-1.712	89.731	1.00 14.65	A
	ATOM	2510	CZ	TYR	352	25.989	-1.180	90.848	1.00 15.26	A
			OH	TYR	352			90.715	1.00 17.76	A
15	ATOM	2511				26.767	-0.050			
45	ATOM	2512	С	TYR	352	24.688	-5.973	92.733	1.00 16.43	A
	ATOM	2513	0	TYR	352	25.917	-5.964	92.715	1.00 17.51	A
	MOTA	2514	N	ALA	353	23.989	-6.065	93.855	1.00 15.81	A
	ATOM	2515	CA	ALA	353	24.658	-6.137	95.145	1.00 16.65	A
	ATOM	2516	CB	ALA	353	23.646	-5.931	96.269	1.00 15.23	A
50										
50	MOTA	2517	С	ALA	353	25.405	-7.458	95.350	1.00 17.40	A
	ATOM	2518	0	ALA	353	26.412	-7.497	96.050	1.00 18.96	A
	MOTA	2519	N	HIS	354	24.916	-8.535	94.744	1.00 18.26	A
	ATOM	2520	CA	HIS	354	25.555	-9.838	94.883	1.00 19.76	A
	MOTA	2521	СВ	HIS	354	24.676	-10.932	94.266	1.00 19.50	A
55	MOTA	2522	CG	HIS	354	25 1/13	-12.324	94.566	1.00 21.21	A
00										
	MOTA	2523	CDZ	HIS	354	25.758	-13.246	93.786	1.00 20.11	A
	ATOM	2524	ND1	HIS	354	25.032	-12.894	95.817	1.00 20.61	A
	ATOM	2525		HIS	354		-14.105	95.796	1.00 20.62	A
	ATOM	2526	NEZ	HIS	354	26.009	-14.342	94.576	1.00 20.83	A
60	MOTA	2527	С	HIS	354	26.936	-9.842	94.224	1.00 21.08	A
		2528		HIS	354				1.00 22.05	A
	MOTA		-							
	MOTA	2529	N	ARG	355	27.027	-9.314	93.004	1.00 22.49	A
	ATOM	2530	CA	ARG	355	28.308	-9.256	92.292	1.00 24.62	A
15	MOTA	2531	CB	ARG	355	28.153	-8.619	90.905	1.00 25.83	A
65	MOTA	2532	CG	ARG	355	27.358	-9.413	89.894	1.00 29.38	Α
	MOTA	2533	CD	ARG	355	27.482	-8.762	88.535	1.00 32.38	A
	MOTA	2534	NE	ARG	355	27.233	-7.326	88.622	1.00 37.22	A
	MOTA	2535	CZ	ARG	355	27.902	-6.412	87.924	1.00 40.93	A
70	MOTA	2536		ARG	355	28.860	-6.79 7	87.087	1.00 41.58	A
70	MOTA	2537	NH2	ARG	355	27.624	-5.117	88.066	1.00 39.72	A
-		2538	С	ARG	355	29.352	-8.447	93.054	1.00 24.34	A
	MOTA									
	MOTA	2539	0	ARG	355	30.523	-8.821	93.098	1.00 25.69	A
	MOTA	2540	N	ALA	356	28.923	-7.332	93.640	1.00 23.36	A

	ATOM	2541	CA	ALA	356	29.814	-6.447	94.387	1.00 22.82	A
	MOTA	2542	CB	ALA	356	29.016	-5.295	94.985	1.00 20.20	A
	ATOM	2543	С	ALA	356	30.603	-7.161	95.484	1.00 23.12	A
_	MOTA	2544	0	ALA	356	31.708	-6.751	95.820	1.00 20.69	A
5	MOTA	2545	N	LYS	357	30.030	-8.222	96.047	1.00 24.95	A
	ATOM	2546	CA	LYS	357	30.695	-8.981	97.111	1.00 26.72	A
	MOTA	2547	CB	LYS	357	29.849	-10.195	97.497	1.00 25.95	A
	ATOM	2548	CG	LYS	357	28.570	-9.854	98.232	1.00 27.20	A
	MOTA	2549	CD	LYS	357		-11.052	98.293	1.00 28.41	A
10	ATOM	2550	CE	LYS	357		-12.220	99.024	1.00 29.67	A
	ATOM	2551	NZ	LYS	357		-13.483	98.790	1.00 30.65	 A
	ATOM	2552	c	LYS	357	32.099	-9.453	96.733	1.00 27.68	Ä
	MOTA	2553	ŏ	LYS	357	32.968	-9.595	97.601	1.00 26.10	A.
	ATOM	2554	N	ASN	358	32.312	-9.691	95.438	1.00 28.56	A
15	ATOM	2555	CA	ASN	358		-10.177	94.925	1.00 28.98	A
	ATOM	2556	CB	ASN	358		-10.897	93.597	1.00 31.13	Ä
	MOTA	2557	CC	ASN	358		-12.071	93.735	1.00 34.60	Ä
	MOTA			ASN			-13.071			
	MOTA	2558 2559	ND2		358 358			94.375	1.00 37.20	A
20							-11.952	93.145	1.00 33.97	A
20	MOTA	2560	c	ASN	358	34.676	-9.118	94.751	1.00 27.98	A
	MOTA	2561	0	ASN	358	35.784	-9.426	94.316	1.00 28.50	A
	MOTA	2562	N	ILE	359	34.364	-7.871	95.079	1.00 25.92	A
	MOTA	2563	CA	ILE	359	35.350	-6.811	94.957	1.00 24.09	A
25	MOTA	2564	CB	ILE	359	34.673	-5.429	94.910	1.00 21.25	A
25	MOTA	2565		ILE	359	35.727	-4.329	94.867	1.00 19.17	A
	ATOM	2566		ILE	359	33.748	-5.367	93.689	1.00 19.08	A
	ATOM	2567		ILE	359	32.909	-4.109	93.597	1.00 18.25	A
	ATOM	2568	С	ILE	359	36.290	-6.906	96.155	1.00 25.26	A
20	MOTA	2569	0	ILE	359	35.847	-7.076		1.00 23.96	A
30	MOTA	2570	N	LEU	360	37.588	-6.817	95.897	1.00 27.58	A
	ATOM	2571	CA	LEU	360	38.578	-6.917	96.963	1.00 32.07	A
	ATOM	2572	CB	LEU	360	39.478	-8.137	96.722	1.00 34.40	A
	MOTA	2573	CG	LEU	360	40.711	-8.333	97.613	1.00 36.57	A
25	ATOM	2574	CD1	LEU	360	40.309	-8.930	98.951	1.00 37.87	A
35	ATOM	2575	CD2	LEU	360	41.687	-9.265	96.913	1.00 38.48	A
	MOTA	2576	С	LEU	360	39.438	-5.665	97.033	1.00 33.54	A
•	MOTA	2577	0	LEU	360	39.905	-5.174	96.008	1.00 32.97	A
	ATOM	2578	N	ASN	361	39.635	-5.132	98.234	1.00 35.62	A
	MOTA	2579	CA	ASN	361	40.485	-3.962	98.372	1.00 39.86	A
40	ATOM	2580	CB	ASN	361	39.649	-2.672	98.395	1.00 41.32	A
	ATOM	2581	CG	ASN	361	38.490	-2.732	99.345	1.00 42.28	A
	MOTA	2582	OD1	ASN	361	37.523	-1.985	99.203	1.00 42.60	A
	ATOM	2583	ND2	ASN	361	38.578	-3.609	100.330	1.00 45.41	A
	MOTA	2584	C	ASN	361	41.439	-4.056	99.565	1.00 41.68	A
45	ATOM	2585	0	ASN	361	41.180		100.532	1.00 41.90	A
	ATOM	2586.	N'	LYS	362	42.560	-3.348	99.446	1.00 44.89	A
	ATOM	2587	CA	LYS	362	43.643		100.432	1.00 46.74	A
	MOTA	2588	CB	LYS	362	43.106		101.870	1.00 45.91	A
	ATOM	2589	CG	LYS	362	42.518		102.353	1.00 44.95	A
50	MOTA	2590	CD	LYS	362	42.184		103.841	1.00 44.77	\ A
	ATOM	2591	CE	LYS	362	43.444		104.701	1.00 44.68	A
	ATOM	2592	NZ	LYS	362	44.224		104.523	1.00 44.09	A
	MOTA	2593	¢	LYS	362	44.576		100.173	1.00 48.88	 A
	MOTA	2594	ŏ	LYS	362	44.928		101.141	1.00 50.91	Ä
55	ATOM	2595	OXT		362	44.955	-4.700	98.992	1.00 49.21	A A
	ATOM	2596	MG	HG	603	16.038	9.381	98.154	1.00 22.45	
	MOTA	2597	PB	ADP	601	14.871	6.512	98.896	1.00 9.83	ADP
	MOTA	2598	01B		601	14.389	7.073	97.604	1.00 11.43	ADP
	ATOM	2599	02B		601	15.417	5.029	98.682	1.00 12.43	ADP
60	ATOM	2600	03B			15.921	7.374			
00					601			99.491	1.00 9.54	ADP
	ATOM	2601	PA		601	13.343		101.254	1.00 13.34	ADP
	MOTA	2602	01A		601	14.336		102.280	1.00 14.02	ADP
	ATOM	2603	02A		601	13.336		101.013	1.00 12.22	ADP
65	MOTA	2604	03A		601	13.676	6.373	99.912	1.00 11.56	ADP
J.J	MOTA	2605	05*		601	11.879		101.742	1.00 16.31	ADP
	MOTA	2606	C5*		601	10.894		101.155	1.00 16.15	ADP
	MOTA	2607	C4.		601	9.662		102.132	1.00 18.96	ADP
	MOTA	2608	04 *		601	9.712		102.849	1.00 19.62	ADP
70	ATOM	2609	C3 •		601	9.700		103.229	1.00 18.60	ADP
70	MOTA	2610	03*		601	8.406		103.431	1.00 22.72	ADP
	MOTA	2611	C2*		601	10.188		104.496	1.00 19.66	ADP
	MOTA	2612	02 *		601	9.655		105.672	1.00 21.78	ADP
	ATOM	2613	C1.	ADP	601	9.788	4.947	104.281	1.00 19.08	ADP

	MOTA	2614	и9	ADP	601	10.778		104.795	1.00 19.36	ADP
	MOTA	2615	C8	ADP	601	11.895	3.536	104.137	1.00 19.33	ADP
	ATOM	2616	N7	ADP	601	12.535	2.641	104.859	1.00 19.29	ADP
	ATOM	2617	C5	ADP	601	11.874		105.961	1.00 20.60	ADP
5	ATOM	2618	C6	ADP	601	12.043		107.091	1.00 20.38	ADP
5									1.00 20.28	
	MOTA	2619	N6	ADP	601	13.085		107.178		ADP
	MOTA	2620	N1	ADP	601	11.118		108.120	1.00 22.79	ADP
	MOTA	2621	C2	ADP	601	10.028	2.524	108.081	1.00 22.78	ADP
	MOTA	2622	N3	ADP	601	9.854	3.302	106.988	1.00 20.98	ADP
10	ATOM	2623	C4	ADP	601	10.736	3.301	105.936	1.00 20.39	ADP
	ATOM	2859	C1	5-2b	2	19.000	14.175		1.00 28.18	5-2b
	MOTA	2860	C2	5-2b	2		13.539		1.00 32.48	5-2b
						18.061				
	MOTA	2861	C3	5-2b	2	17.078		111.895	1.00 28.56	5-2b
	MOTA	2862	C4	5-2b	2	17.088	12.427		1.00 27.05	5-2b
15	MOTA	2863	C5	5-2b	2	18.039	13.044	114.157	1.00 26.16	5-2b
	MOTA	2864	C6	5-2b	2	19.015	13.950	113.622	1.00 28.62	5-2b
	ATOM	2865	C7	5-2b	2	18.128	13.723	109.878	1.00 39.58	5-2b
	ATOM	2866	N8	5-2b	2	19.295	13.211		1.00 34.03	5-2b
		2867	C9	5-2b	2	20.221	14.007		1.00 31.92	5-2b
20	MOTA									
20	ATOM	2868		5-2b	2	19.947	15.297		1.00 36.78	5-2b
	ATOM	2869		5-2b	2	18.661	15.862		1.00 44.76	5-2b
	MOTA	2870	C12	5-2b	2	17.708	15.078	109.368	1.00 52.53	5-2b
	MOTA	2871	013	5-2b	2	16.238	11.708	113.800	1.00 23.44	5-2b
	ATOM	2872	C14	5-2b	2	16.264	15.498		1.00 70.42	·5-2b
25	MOTA	2873	015	5-2b	2	15.927	16.837		1.00104.53	5-2b
		2874			2					5-2b
	MOTA			5-2b		14.579	17.475		1.00 95.04	
	MOTA	2875	C17		2.	14.646	19.021		1.00 97.91	5-2b
	MOTA	2876		5-2b	2	18.590	17.336		1.00 43.13	5-2b
	MOTA	2877	019	5-2b	2	15.462	14.612	109.721	1.00 72.50	5-2b
30	MOTA	2878	S20	5-2b	2	21.688	13.451	108.038	1.00 18.17	5-2b
	MOTA	2624	0	нон	1	20.805	10.444	96.618	1.00 3.59	S
	ATOM	2625	ō	нон	6	18.478	8.895	97.954	1.00 22.75	s
	MOTA	2626	ŏ	нон	7	8.678	16.203		1.00 5.86	Š
				нон						s
35	ATOM	2627	0		8	15.946	-1.691	94.899	1.00 5.80	
ככ	ATOM	2628	0	нон	11	21.220	17.072		1.00 1.72	s
	MOTA	2629	0	HOH	13	14.805	10.449	99.917	1.00 8.07	S
	MOTA	2630	0	HOH	16	13.355	~2.493	95.064	1.00 7.03	S
	ATOM	2631	0	HOH	19	21.262	3.695	111.999	1.00 8.18	s
	ATOM	2632	Ō	нон	20	10.684	13.846		1.00 18.83	s
40	MOTA	2633	ō		, 25	21.216	2.976	93.758	1.00 14.00	s
70										s
	MOTA	2634	0	нон	27	24.932	11.371		1.00 7.13	
	MOTA	2635	0	нон	34	15.711	22.783		1.00 8.16	s
	ATOM	2636	0	нон	35	31.658	6.477	79.773	1.00 16.68	S
	ATOM	2637	0	HOH	36	16.262	7.930	95.115	1.00 13.14	S
45	ATOM	2638	0	нон	38	15.341	-0.450	103.081	1.00 3.96	S
	MOTA	2639	0	нон	40	20.527	12.061		1.00 13.66	S
	MOTA	2640	ŏ	нон	42	31.548	4.510	82.184	1.00 13.63	s
		2641						109.317		Š
	ATOM		0	нон	44	20.139				
50	MOTA	2642	0	нон	46	38.748		117.615	1.00 16.12	S
50	MOTA	2643	0	нон	48	37.332	6.832	98.871	1.00 20.54	S
	MOTA	2644	0	нон	50	15.243	1.107	105.237	1.00 7.71	s
	MOTA	2645	0	нон	52	23.362	13.594	103.308	1.00 16.03	S
	ATOM	2646	0	нон	54	24.373	1.678	79.508	1.00 21.19	s
	MOTA	2647	0	нон	55	38.272	4.890	80.366	1.00 15.34	s
55	ATOM	2648	ŏ	нон	60	28.231	24.639	95.411	1.00 10.59	s
55										
	MOTA	2649	0	нон	61	39.120	8.121	96.836	1.00 17.30	S
	MOTA	2650	0	нон	63	18.805	15.804		1.00 24.81	S
	ATOM	2651	0	нон	64	40.943	11.048	89.550	1.00 24.53	S
	MOTA	2652	0	HOH	68	31.035	20.952	88.723	1.00 17.53	S
60	MOTA	2653	0	нон	69	19.610	-3.671	118.241	1.00 28.77	S
	MOTA	2654	ō	нон	70	23.256		117.749		Š
	ATOM								1.00 12.03	
		2655	0	HOH	71	21.279	14.920		1.00 17.07	S
	ATOM	2656	0	нон	72	11.571	8.465	98.099	1.00 17.54	S
	MOTA	2657	0	нон	73	0.219	-7.157	96.638	1.00 36.34	S
65	ATOM	2658	0	нон	74	14.061	-2.365	107.352	1.00 17.49	s
	MOTA	2659	0	нон	75	38.428		101.400	1.00 20.61	S
	ATOM	2660	ò	нон	76	28.147	6.297	79.763	1.00 6.93	S
	MOTA	2661	ŏ	нон	78		-15.702		1.00 42.69	š
	MOTA	2662	ŏ	нон	79		11.793			S
70						40.740		96.499	1.00 19.31	
10	MOTA	2663	0	нон	82	38.334	-6.005		1.00 25.92	s
	MOTA	2664	0	нон	83	28.296	. 4.768	77.136	1.00 31.56	S
	ATOM	2665	0.	нон	84	14.008	16.450	94.704	1.00 5.75	S
	MOTA	2666	0	нон	87	45.629		110.783	1.00 17.29	s
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	MOTA	2667	0	нон	90	13.592		92.309	1.00 13.66	S
	MOTA	2668	0	нон	91	9.122	2.181	96.091	1.00 36.98	S
	MOTA	2669	0	нон	92	16.369	12.885	106.048	1.00 20.85	S
	MOTA	2670	Ō	нон	93	13.386		89.915	1.00 17.97	5
5	ATOM					11.913				
,		2671	0	нон	94		22.331	96.952	1.00 21.35	S
	MOTA	2672	0	нон	95	20.093		89.951	1.00 16.99	s
	ATOM	2673	0	нон	96	17.551	-0.999	87.296	1.00 26.38	S
	ATOM	2674	0	HOH	97	20.767	15.478	84.877	1.00 51.52	S
	ATOM	2675	ō	нон	99	35.477		79.785	1.00 19.87	Š
10										
10	MOTA	2676	0	нон	101	21.955		118.594	1.00 28.07	S
	MOTA	2677	0	нон	102	40.041	5.064	84.678	1.00 16.03	S
	MOTA	267B	0	нон	104	36.377	-3.662	102.275	1.00 18.75	S
	MOTA	2679	0	HOH	106	3.852	11.665	120.058	1.00 30.71	S
	ATOM	2680	Ó	HOH	108	39.673	-0.150	74.200	1.00 46.52	S
15	MOTA	2681	ŏ	. нон	110		-12.000		1.00 50.82	s
13								92.235		3
	MOTA	2682	0	нон	111	30.628		102.526	1.00 21.67	S
	MOTA	2683	0	нон	112	30.065	26.389	96.506	1.00 17.19	S
	MOTA	2684	0	нон	113	14.004	8.985	104.371	1.00 25.20	s
	MOTA	2685	0	нон	114	33.791		74.652	1.00 19.53	s
20	ATOM	2686	ō	нон	117	22.111		120.746	1.00 38.73	Š
20										
	ATOM	2687	0	нон	118	26.607		84.656	1.00 17.38	S
	MOTA	2688	0	HOH	121	21.035	-9.445	110.275	1.00 13.05	s
	MOTA	2689	0	нон	122	32.184	14.826	101.349	1.00 11.39	S
	MOTA	2690	0	нон	123	17.599	-1.616	90.813	1.00 13.59	S
25	ATOM	2691	0	нон	124	34.130		110.137	1.00 23.55	s
		2692	ŏ	нон						. s
	ATOM				126	9.990		95.389	1.00 15.79	
	MOTA	2693	0	HOH	129		-12.862	94.601	1.00 59.83	S
	MOTA	2694	0	нон	130	13.955	10.696	95.694	1.00 19.43	s
	ATOM	2695	0	нон	131	31.703	25.858	98.664	1.00 24.88	s
30	MOTA	2696	0	нон	132	35.057	22.912	85.606	1.00 40.74	S
	ATOM	2697	ō	нон	134	15.475	-7.722	86.631	1.00 12.20	s
	ATOM	2698	0	нон	135	17.594		102.663	1.00 23.55	S
	ATOM	2699	0	нон	136	7.395	-14.251	99.064	1.00 49.69	s
~-	MOTA	2700	0	нон	137	16.245	22.597	107.873	1.00 19.89	s
35	MOTA	2701	0	нон	139	9.431	-0.664	90.038	1.00 31.01	S
	MOTA	2702	0	нон	145	19.183		93.555	1.00 40.54	s
	MOTA .	2703	ŏ	нон	146	27.383		122.250	1.00 22.34	Š
	MOTA	2704	0	нон	148	39.078	-6.174	93.184	1.00 34.51	S
40	MOTA	2705	0	HOH	149	49.726	3.941	96.574	1.00 41.42	s
40	MOTA	2706	0	нон	151	13.531	20.213	113.505	1.00 35.47	s
	MOTA	2707	٥	HOH	152	49.848	18.275	102.636	1.00 39.85	S
	MOTA	2708	0	нон	153	27.728		103.176	1.00 32.11	s
	MOTA	2709	ō	нон	154	17.610	7.968	89.633	1.00 32.29	s
45	MOTA	2710	0	HOH	155	16.723	19.937	85.776	1.00 24.59	·s
43	MOTA	2711	0	нон	158	31.015	-3.720	75.821	1.00 31.57	S
	MOTA	2712	0	нон	159	39.461	15.014	103.524	1.00 34.83	s
	MOTA	2713	0	нон	164	45.236	2.614	116.065	1.00 33.66	s
	ATOM	2714	0	нон	166	28.893		123.561	1.00 30.64	s
	ATOM	2715	ō	нон	167	35.887	12.107	99.622	1.00 11.12	s
50										
50	MOTA	2716	0	нон	168	29.323	-10.874		1.00 39.92	S
	ATOM	2717	0	нон	170	33.078		122.206	1.00 27.20	S
	MOTA	2718	0	нон	171	6.377	-23.385	91.461	1.00 39.35	S
	MOTA	2719	٥	нон	175	38.059	24.742	100.957	1.00 44.52	S
	MOTA	2720	0	нон	179	12.119		109.488	1.00 28.60	s
55	ATOM	2721	ŏ	нон	184	35.206		104.290	1.00 21.93	s
	ATOM .	2722	Ö							
				нон	186	5.690	-6.930	88.872	1.00 26.18	S
	MOTA	2723	0	HOH	187		-13.329		1.00 25.44	S
	ATOM	2724	0	нон	188	8.547	-5.057	88.499	1.00 31.53	s
	MOTA	2725	٥	HOH	189	13.396	13.012	123.817	1.00 23.03	S
60	ATOM	2726	ō	нон	190	37.857	10.497	99.808	1.00 16.10	Š
	MOTA	2727	ŏ						1.00 32.35	s
			-	нон	191	15.390			2.00 00.00	_
	MOTA	2728	0	нон	192	24.877	12.484	84.150	1.00 33.77	. S
	MOTA	2729	0	нон	195	7.560		103.939	1.00 24.38	s
	MOTA	2730	0	HOH	197	38.275	6.762	75.942	1.00 34.75	s
65	MOTA	2731	0	нон	198	11.981		109.242	1.00 26.93	s
	MOTA	2732	ŏ	нон	199		-13.318	94.699	1.00 32.78	s
									_	
	MOTA	2733	0	нон	201	33.413			1.00 31.96	S
	ATOM .	2734	0	HOH	203	25.859	12.342	87.393	1.00 39.56	S
	ATOM	2735	0	HOH	205	21.304	4.617	78.647	1.00 17.67	s
70	MOTA	2736	0	нон	207	23.255	12.937	88.372	1.00 28.66	S
	MOTA	2737	ŏ	нон	208	7.965	2.363	93.256	1.00 39.90	s
									1.00 39.55	
	MOTA	2738	0	HOH	210		-19.119	97.337		S
	MOTA	2739	0	нон	211	23.200	15.157	105.669	1.00 3.65	S

	MOTA	2740	0	нон	212	16.820	11.748	98.364	1.00 4.40	S
	MOTA	2741	0	нон	215	37.029	15.874	102.172	1.00 9.34	S
	MOTA	2742	0	нон	217	45.218	10.237	90.158	1.00 50.32	S
	ATOM	2743	Ó	нон	220	46.617		108.402	1.00 29.26	S
-5	MOTA	2744	ŏ	нон	221	18.955		95.378	1.00 23.41	Š
9										
	MOTA	2745	0	нон	223	22.905			1.00 15.81	S
	MOTA	2746	0	нон	225	2.959		97.196	1.00 46.93	S
	MOTA	2747	0	нон	226	11.436	16.916	109.490	1.00 15.86	s
	MOTA	2748	0	HOH	228	16.698	14.117	102.916	1.00 25.42	S
10	ATOM	2749	0	нон	229	14.674		106.079	1.00 26.44	S
	ATOM	2750	ō	нон	232	21.595		87.827	1.00 14.15	s
-	ATOM	2751	ŏ	нон						
					233	11.151		115.185	1.00 32.57	s
	MOTA	2752	0	HOH	238	29.371		77.740	1.00 19.94	S
	MOTA	2753	0	нон	241	13.508	12.891	99.625	1.00 20.34	S
15	MOTA	2754	0	нон	243	17.423	4.974	118.567	1.00 24.32	s
	MOTA	2755	0	нон	244	21.246	6.736	82.924	1.00 39.07	S
	ATOM	2756	0	нон	245	11.590		98.284	1.00 19.24	S
	ATOM	2757	ō	нон	247	51.802		117.095	1.00 55.38	s
	MOTA	2758	ŏ	нон	251				1.00 31.61	
20						8.180		99.128		S
20	MOTA	2759	0	нон	252	21.300		98.575	1.00 31.29	S
	MOTA	2760	0	HOH	253	41.894		97.607	1.00 30.47	s
	MOTA	2761	0	нон	254	23.625	0.733	121.375	1.00 27.92	S.
	ATOM	2762	0	нон	255	29.438	14.355	123.667	1.00 26.17	S
	ATOM	2763	0	нон	256	20.446		116.657	1.00 34.15	·s
25	MOTA	2764	ō	нон	257	11.975		91.516	1.00 18.84	s
	MOTA	2765	ō	нон						
					260	13.789		113.975	1.00 23.75	S
	ATOM	2766	0	нон	262	7.623		124.008	1.00 30.74	S
	MOTA	2767	0	нон	263	20.395		81.694	1.00 33.87	S
20	MOTA	2768	0	нон	266	34.255	-0.467	81.343	1.00 30.08	s
30	MOTA	2769	0	нон	268	45.417	1.198	105.917	1.00 33.79	S
	MOTA	2770	0	нон	271	15.540	-18.971	104.185	1.00 36.81	S
	MOTA	2771	0	нон	272	31.560		95.365	1.00 25.41	s
	MOTA	2772	ō	нон	273	10.820		124.773	1.00 27.96	S
		2773								
35	ATOM		0	HOH	275	16.259		106.228	1.00 15.83	s
33	MOTA	.2774	0	нон	279	14.255		104.198	1.00 21.24	S
	MOTA	2775	0	нон	280	14.152	22.369	109.944	1.00 30.26	s
	MOTA	2776	0	нон	281	28.645	-13.914	110.927	1.00 35.08	s
	ATOM	2777	0	HOH	283	15.855	18.951	102.400	1.00 31.06	S
	ATOM	2778	0	нон	288	15.557		116.261	1.00 19.13	S
40	ATOM	2779	ŏ	нон	290	52.550		99.218	1.00 47.57	s
	ATOM	2780	ŏ	нон						
					291	26.202		81.794	1.00 53.97	S
	MOTA	2781	0	нон	294	20.086		120.312	1.00 37.20	S
	MOTA	2782	0	нон	295	6.012		120.875	1.00 18.20	S
4.5	MOTA	2783	0	HOH	296	30.916	30.335	103.939	1.00 37.71	S
45	MOTA	2784	0	нон	297	46.048	18.195	120.452	1.00 43.25	S
	MOTA	2785	0	нон	299	31.569		101.042	1.00 32.15	S
	MOTA	2786	ō	нон	300	21.162	-3.401	87.125	1.00 32.61	s
	ATOM	2787	ŏ	нон	303	9.761		112.502	1.00 27.58	S
50	ATOM	2788	0	нон	305	32.066		112.422	1.00 32.24	S
50	MOTA	2789	0	HOH	307	33.480	-2.576	83.015	1.00 27.49	S
	MOTA	2790	0	нон	308	2.984	13.923	120.708	1.00 31.57	s
	MOTA	2791	0	нон	309	34.596	-15.790	94.772	1.00 43.06	S
	MOTA	2792	0	HOH	310	34.476	-4.326	104.147	1.00 46.76	s
	ATOM	2793	ō	нон	313	18.109	-9.045	87.036	1.00 25.07	s
55	ATOM	2794	ŏ	нон				121.659	1.00 42.28	
					314	2.837				S
	ATOM	2795	0	HOH	315	13.698	1.784	111.141	1.00 35.74	S
	MOTA	2796	0	нон	317	34.111	18.005	122.006	1.00 28.52	s
	ATOM	2797	0	нон	318	29.111	-3.283	83.701	1.00 38.21	s
	ATOM	2798	0	нон	319	32.667	0.553	105.431	1.00 27.32	s
60	MOTA	2799	0	HOH	323	4.556	-19.468	88.447	1.00 56.20	s
	MOTA	2800	ō	нон	324	-2.283		97.004	1.00 48.36	Š
	ATOM	2801								
			0	нон	327	28.636		118.234	1.00 30.32	S
	MOTA	2802	0	нон	328	29.441		120.010	1.00 30.29	S
60	MOTA	2803	0	нон	331	25.024	1.315	88.662	1.00 35.16	S
65	MOTA	2804	0	HOH	332	25.076	33.728	92.315	1.00 37.36	s
	MOTA	2805	0	HOH	334	17.967	17.125	84.628	1.00 44.99	s
	MOTA	2806	ŏ	нон	336	35.277	-4.775	82.255	1.00 22.90	S
	MOTA	2807	ŏ	нон	338					S
		2808				5.655	-0.231	95.494	1.00 39.33	
70	MOTA		0	нон	340	46.414		108.144	1.00 58.72	s
70	ATOM	2809	0	нон	342	10.262	-2.840	88.835	1.00 36.82	S
	MOTA	2810	0	нон	344	48.378	-0.812	102.187	1.00 39.43	s
	ATOM	2811	0	HOH	345	7.840	6.837	118.967	1.00 54.06	s
	ATOM	2812	0	нон	347	42.036	-0.811	90.785	1.00 34.08	Š
					- • .	32.030	021			-

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	MOTA	2813	0	нон	351	51.775	6.542	133.541	1.00 37.45	S
	ATOM	2814	0	HOH	354	31.545	13.101	83.668	1.00 37.78	s
	MOTA	2815	0	HOH	355	35.526	14.686	100.364	1.00 8.84	S
_	MOTA	2816	0	нон	361	12.290	20.796	107.012	1.00 17.59	s
5	MOTA	2817	0	нон	363	40.627	4.272	127.391	1.00 41.84	s
	MOTA	2818	0	HOH	365	30.371	-1.879	79.833	1.00 13.67	S
	ATOM	2819	0	нон	367	11.687	18.291	107.264	1.00 22.06	s
	MOTA	2820	0	нон	370	18.511	7.004	119.773	1.00 38.47	S
	ATOM	2821	0	нон	371	17.908		100.054	1.00 12.12	s
10	ATOM	2822	0	нон	372	27.131	-3.005	76.310	1.00 16.74	s
	MOTA	2823	0	нон	375	8,972	7.52B	97.923	1.00 26.11	S
	MOTA	2824	ò	нон	377	18.727	10.788	84.519	1.00 41.33	S
	ATOM	2825	o	нон	379	14.127	15.750	98.863	1.00 25.29	S
	MOTA	2826	ō	нон	383	41.700	9.858	81.807	1.00 33.52	Š
15	MOTA	2827	Ó	нон	385	35.261		106.016	1.00 28.87	s
	ATOM	2828	ō	нон	386	12.726		115.689	1.00 46.81	S
	MOTA	2829	ō	HOH	393	43.648		106.741	1.00 16.47	Š
	ATOM	2830	ō	нон	394	37.259		104.054	1.00 14.17	Š
	MOTA	2831	ō	HOH	396	24.282	-6.502	87.829	1.00 42.62	Š
20	ATOM	2832	ō	нон	400	43.027	-3.036	92.095	1.00 34.87	Š
	ATOM	2833	ō	нон	406	31.066	-3.244	81.803	1.00 24.95	Š
	ATOM	2834	ō	нон	409	36.251		119.019	1.00 19.28	S
	MOTA	2835	ō	нон	415	10.534		100.073	1.00 39.35	Š
	ATOM	2836	ŏ	нон	418	8.054		110.289	1.00 45.64	s
25	ATOM	2837	ŏ	нон	422	39.306		111.576	1.00 34.28	Š
	ATOM	2838	ō	нон	425	6.396		103.157	1.00 32.56	Š
	ATOM	2839	ō	нон	426	39.952	24.546	98.144	1.00 27.08	s
	MOTA	2840	ō	нон	429	39.863	6.685	82.133	1.00 40.09	s
	MOTA	2841	õ	нон	430	21.921	12.487	85.799	1.00 40.68	Š
30	ATOM	2842	ō	нон	433	11.505		100.809	1.00 30.56	Š
	ATOM	2843	ō	нон	435	10.302		104.901	1.00 29.96	S
	MOTA	2844	ō	нон	438	23.476	-0.876	78.128	1.00 28.68	S
	ATOM	2845	ō	нон	442	40.869		100.914	1.00 39.98	Š
	ATOM	2846	ō	нон	444	36.147	28.207	94.921	1.00 46.43	s
35	MOTA	2847	ō	нон	445	23.713		119.077	1.00 42.21	s
	ATOM	2848	ō	нон	447	27.306	-4.631	90.698	1.00 43.77	Š
	ATOM	2849	ō	нон	448	45.805		107.875	1.00 28.04	S
	ATOM	2850	ō	нон	449	11.162		125.577	1.00 42.08	s
	ATOM	2851	ō	нон	450	51.897		132.993	1.00 37.33	s
40	ATOM	2852	ŏ	нон	452	28.491		119.002	1.00 32.94	Š
	ATOM	2853	ō	нон	454	8.173		105.141	1.00 50.50	š
	ATOM	2854	ŏ	нон	459	42.750	5.736	87.519	1.00 36.93	s
	ATOM	2855	ŏ	нон	460	30.376	34.460	94.131	1.00 31.43	S
	ATOM	2856	ŏ	нон	466	25.986		120.060	1.00 52.81	Š
45	ATOM	2857	ŏ	нон	467		-10.959		1.00 29.27	S
-	ATOM	2858	ō	нон	468	23.362	-2.077	86.180	1.00 37.76	S
	END		-			22.502	2.477	30.200		-

TABLE 2

	DDWADE	,	C	. د	1 7 7 2	.b2b1) a D			
	REMARK !CRYST		.250			b.pdb molec		0.00 90.00	P212121	
5	ATOM	20	СВ	LYS	17	24.352			1.00 51.00	В
	MOTA	21	CG	LYS	17	22.874			1.00 53.34	В
	MOTA	22	CD	LYS	17	22.663			1.00 53.77	В
	MOTA	23	CE	LYS	17	23.197			1.00 54.85	В
10	MOTA	24	NZ	LYS	17		-13.69		1.00 53.86	В
10	MOTA	25	C	LYS	17 17		-10.10		1.00 47.83	B B
	ATOM ATOM	26 27	O N	LYS LYS	17	25.275 24.345			1.00 48.69	В
	ATOM	28	CA	LYS	17	24.911	-11.04		1.00 49.15	В
	MOTA	29	N	ASN	18	23.597	-9.26		1.00 45.98	В
15	ATOM	30	CA	ASN	18	23.245	-8.34		1.00 43.66	В
	ATOM	31	CB	ASN	18	21.960	-7.62	27 58.880	1.00 45.49	В
	MOTA	32	CG	ASN	18	20.740	-8.48		1.00 49.80	В
	ATOM	33		ASN	18	20.453	-8.81		1.00 50.22	В
20	ATOM ATOM	34 35	ND2 C	asn asn	18 18	20.019 24.338	-8.85 -7.33		1.00 49.94	B B
20	ATOM	36	ō	ASN	18	24.671	-7.17		1.00 41.62	₿.
	ATOM	37	N	ILE	19	24.906	-6.66		1.00 37.77	. B
	ATOM	38	CA	ILE	19	25.949	-5.67		1.00 34.25	В
~~	MOTA	39	CB	ILE	19	26.325	-4.96		1.00 35.25	В
25	MOTA	40		ILE	19	26.548	-5.98		1.00 38.29	В
	MOTA	41		ILE	19	27.581	-4.13		1.00 35.22	В
	MOTA MOTA	42 43	CDI	ILE	19 19	28.042 27.213	-3.48 -6.27		1.00 36.16	B B
	MOTA	44	Ö	ILE	19	27.730	-7.28		1.00 31.52	В
30	ATOM	45	N	GLN	20	27.699	-5.63		1.00 27.50	B
	ATOM	46	CA	GLN	20	28.903	~6.09		1.00 26.14	В
	MOTA	47	CB	GLN	20	28.889	-5.60		1.00 25.10	В
	MOTA	48	CG	GLN	20	30.276	-5.49		1.00 27.01	В
35	MOTA	49	CD	GLN	20	30.232	-5.16		1.00 29.81	В
22	MOTA MOTA	50 51	OE1 NE2	GLN GLN	20 20	29.920 30.546	-6.02 -3.92		1.00 30.67 1.00 30.62	B B
	ATOM	52	C	GLN	20	30.162	-5.56		1.00 30.62	В
	MOTA	53	õ	GLN	20	30.211	-4.39		1.00 27.09	В
	MOTA	54	N	VAL	21	31.176	-6.42	26 57.327	1.00 22.08	В
40	MOTA	55	CA	VAL	21	32.427	-6.04	18 57.989	1.00 18.37	В
	ATOM	56	CB	VAL	21	32.472	-6.58		1.00 19.87	В
	MOTA	57 58		VAL VAL	21	33.802	-6.23		1.00 16.85	B B
	MOTA MOTA	59	C	VAL	21 21	31.300 33.648	-6.00		1.00 18.19	В
45	ATOM	60	ō	VAL	21	33.848	-7.77		1.00 16.60	В
	ATOM	61	N	VAL	22	34.457	-5.63		1.00 17.58	В
	MOTA	62	CA-	VAL	22	35.651	-5.96		1.00 15.68	В
	ATOM	63	CB	VAL	22	35.568	-5.38		1.00 17.56	В
50	MOTA MOTA	64 65	CG1	VAL VAL	22 22	34.305 35.553	-5.86 -3.86		1.00 17.79	8 B
50	MOTA	66	C	VAL	22	36.869	-5.39		1.00 17.41	В
	ATOM	67	ŏ	VAL	22	36.746	-4.50		1.00 14.89	В
	ATOM	68	N	VAL	23	38.038	-5.93		1.00 14.83	В
	ATOM	69	CA	VAL	23	39.304	-5.53		1.00 13.82	В
55	ATOM	70	CB	VAL	23	39.935	-6.74		1.00 13.54	В
	MOTA	71	CG1	VAL	23	41.330	-6.40		1.00 6.83	В
	ATOM ATOM	72 73	C	VAL VAL	23 23	39.034 40.304	-7.11 -5.02		1.00 13.12	B B
	MOTA	74	ò	VAL	23	40.414	-5.57		1.00 10.49	В
60	ATOM	75	N	ARG	24	41.008	-3.94		1.00 14.76	В
	ATOM	76	CA	ARG	24	42.019	-3.40		1.00 17.25	В
	ATOM	77	СВ	ARG	24	41.577	-2.08		1.00 14.29	₿
	MOTA	78	CG	ARG	24	42.528	-1.66		1.00 12.98	В
65	MOTA	79	CD	ARG	24	42.331	-0.22		1.00 9.77	В
رن	MOTA	80	NE	ARG	24	42.978	-0.00		1.00 9.97	В
	MOTA MOTA	81 82	CZ NH1	ARG ARG	24 24	42.881 42.165	1.11		1.00 9.72 1.00 3.96	B B
	MOTA	83	NH2		24	43.477	1.17		1.00 3.96	В
	ATOM	84	c	ARG	24	43.328	-3.18		1.00 18.12	В
70	MOTA	85	ō.	ARG	24	43.384	-2.40		1.00 16.79	В
	MOTA	86	N	CYS	25	44.372	-3.87		1.00 21.17	В

	MOTA	87	CA	CYS	25	45.688	-3.764	56.268	1.00 23.23	В
	MOTA	88	CB	CYS	25	46.415	-5.140	56.254	1.00 23.67	В
	MOTA	89	SG	CYS	25	48.096	-5.149	56.970	1.00 28.58	В
	ATOM	90	С	CYS	25	46.464	-2.764	55,443	1.00 24.61	В
5	ATOM	91	ō	CYS	25	46.457	-2.836	54.211	1.00 24.46	В
_					26					
	MOTA	92	N	ARG		47.116	-1.818	56.109	1.00 25.36	В
	MOTA	93	CA	ARG	26	47.897	-0.829	55.380	1.00 27.69	В
	MOTA	94	CB	ARG	26	48.087	0.458	56.219	1.00 26.88	В
	MOTA	95	CG	ARG	26	49.165	0.361	57.300	1.00 25.37	В
10	MOTA	96	CD	ARG	26	49.817	1.722	57.544	1.00 26.81	В
	ATOM	97	NE	ARG	26	51.181	1.599	58.060	1.00 30.34	В
	ATOM	98	cz	ARG	26	51.504	1.598	59.349	1.00 31.91	В
	MOTA	99		ARG	26	50.566	1.721	60.277	1.00 32.84	В
16	MOTA	100		ARG	26	52.767	1.459	59.714	1.00 33.10	В
15	MOTA	101	С	ARG	26	49.268	-1.423	55.072	1.00 29.73	В
	MOTA	102	0	ARG	26	49.673	-2.417	55.676	1.00 28.95	В
	ATOM	103	. N	PRO	27	49.991	-0.832	54.108	1.00 31.27	В
	ATOM	104	CD	PRO	27	49.498	0.108	53.083	1.00 32.66	В
	ATOM	105	CA	PRO	27	51.327	-1.324	53.757	1.00 32.62	В
20										
20	MOTA	106	CB	PRO	27	51.452	-0.937	52.287	1.00 31.65	В
	MOTA	107	CG	PRO	27	50.745	0.369	52.235	1.00 31.82	В
	MOTA	108	С	PRO	27	52.372	-0.626	54.642	1.00 33.24	В
	MOTA	109	0	PRO	27	52.065	0.364	55.311	1.00 33.16	В
•	MOTA	110	N	PHE	28	53.599	-1.141	54.652	1.00 34.79	В
25	MOTA	111	CA	PHE	28	54.670	-0.545	55.451	1.00 34.86	В
	ATOM	112	СВ	PHE	28	55.890	-1.393			В
						55.756	-2.691	55.401	1.00 33.35	
	MOTA	113		PHE	28			56.124	1.00 33.06	В
	MOTA	114		PHE	28	55.856	-3.893	55.440	1.00 31.63	В
20	MOTA	115		PHÉ	28	55.590	-2.715	57.507	1.00 31.31	B
30	MOTA	116	CE1	PHE	28	55.801	-5.102	56.128	1.00 31.40	В
	MOTA	117	CE2	PHE	28	55.536	-3.918	58.193	1.00 30.69	В
	MOTA	118	CZ	PHE	28	55.644	-5.112	57.500	1.00 29.86	В
	MOTA	119	c	PHE	28	55.043	0.842	54.956	1.00 36.62	B
				PHE						
35	MOTA	120	0		28	55.102	1.080	53.752	1.00 36.72	В
23	MOTA	121	N	ASN	29	55.297	1.755	55.885	1.00 39.15	В
	MOTA	122	CA	ASN	29	55.687	3.109	55.517	1.00 43.00	В
	MOTA	123	CB	ASN	29	55.449	4.078	56.693	1.00 41.82	В
	MOTA	124	CG	ASN	29	55.787	3.460	58.044	1.00 41.11	В
	MOTA	125		ASN	29	56.953	3.237	58.367	1.00 38.49	В
40	MOTA	126	ND2		29	54.758	3.178	58.838	1.00 40.06	В
	MOTA	127		ASN	29	57.160	3.083	55.130	1.00 46.95	В
			C							
	MOTA	128	0	ASN	29	57.913	2.236	55.621	1.00 48.65	В
	MOTA	129	N	LEU	30	57.554	3.998	54.243	1.00 49.22	В
	MOTA	130	CA	LEU	30	58.930	4.106	53.751	1.00 49.70	В
45	MOTA	131	CB	LEU	30	59.142	5.490	53.121	1.00 49.24	В
	MOTA	132	CG	LEU	30	60.429	5.757	52.341	1.00 49.29	В
	ATOM	133	CD1		30	60.294	7.104	51.640	1.00 49.07	В
	ATOM	134	CD2		30	61.643	5.740	53.264	1.00 49.24	В
50	MOTA	135	C	LEU	30	59.989	3.866	54.823	1.00 51.07	В
50	MOTA	136	0	LEU	30	60.877	3.032	54.649	1.00 50.68	В
	MOTA	137	N	ALA	31	59.889	4.605	55.925	1.00 52.87	В
	MOTA	138	CA	ALA	31	60.831	4.497	57.035	1.00 54.80	В
	MOTA	139	CB	ALA	31	60.399	5.420	58.157	1.00 53.50	В
	MOTA	140	С	ALA	31	61.011	3.077	57.576	1.00 56.55	В
55	ATOM	141	ŏ	ALA	31	62.140	2.649	57.837	1.00 56.62	В
55										
	MOTA	142	N	GLU	32	59.906	2.354	57.751	1.00 59.00	B
	MOTA	.143	CA	GLU	32	59.958	0.989	58.272	1.00 61.92	В
	MOTA	144	CB	GLU	32	58.625	0.631	58.999	1.00 61.49	В
	MOTA	145	CG	GLU	32	57.413	0.441	58.094	1.00 60.80	В
60	MOTA	146	CD	GLU	32	56.101	0.376	58.872	1.00 59.87	В
	MOTA	147	OE1		32	55.038	0.196	58.242	1.00 58.45	В
	ATOM	148			32	56.129	0.514		1.00 60.23	
			OE2					60.115		В
	ATOM	149	C	GLU	32	60.270	-0.057	57.198	1.00 64.49	В
65	MOTA	150	0	GLU	32	60.610	-1.199	57.522	1.00 64.33	В
65	MOTA	151	N	ARG	33	60.148	0.330	55.927	1.00 67.16	В
	MOTA	152	CA	ARG	33	60.447	-0.573	54.813	1.00 69.70	В
	ATOM	153	CB	ARG	33	59.996	0.033	53.435	1.00 71.95	В
	ATOM	154	CG	ARG	33	58.567	0.570	53.353	1.00 75.31	В
70	MOTA	155	CD	ARG	33	58.383	1.377	52.056	1.00 78.38	В
10	MOTA	156	NE	ARG	33	57.203	2.248	52.066	1.00 80.30	В
	MOTA	157	CZ	ARG	33	56.937	3.167	51.136	1.00 80.67	В
	MOTA	158	NH1	ARG	33	57.766	3.345	50.114	1.00 79.70	В
	MOTA	159	NH2	ARG	33	55.841	3.913	51.226	1.00 80.30	В
						_				-

	MOTA	160	С	ARG	33	61.965	-0.720	54.794	1.00 70.18	. в
	ATOM	161	ō	ARG	33	62.502	-1.813	54.599	1.00 70.13	В
	ATOM	162	Ň	LYS	34	62.638	0.411	54.997	1.00 70.20	В
	MOTA	163	CA	LYS	34	64.094	0.483	55.012	1.00 70.34	В
5	ATOM	164	CB	LYS	34				1.00 70.34	В
,						64.552	1.980	55.063		
	MOTA	165	CG	LYS	34	66.041	2.209	54.795	1.00 71.67	В
	ATOM	166	CD	LYS	34	66.407	3.688	54.868	1.00 71.50	8
	ATOM	167	CE	LYS	34	66.116	4.260	56.251	1.00 72.55	В
10	ATOM	168	NZ	LYS	34	66.513	5.694	56.388	1.00 72.95	₿
10	MOTA	169	С	LYS	34	64.644	-0.288	56.211	1.00 70.18	В
	MOTA	170	0	LYS	34	65.707	-0.915	56.123	1.00 70.68	В
	MOTA	171	N	ALA	35	63.921	-0.236	57.330	1.00 68.80	В
	MOTA	172	CA	ALA	35	64.324	-0.952	58.540	1.00 67.64	В
	MOTA	173	CB	ALA	35	63.605	-0.381	59.760	1.00 67.24	В
15	MOTA	174	С	ALA	35	63.958	-2.424	58.356	1.00 66.54	В
	MOTA	175	0	ALA	35	64.075	-3.232	59.286	1.00 65.43	В
	MOTA	176	N	SER	36	63.520	-2.750	57.138	1.00 64.95	В
	ATOM	177	CA	SER	36	63.113	-4.099	56.770	1.00 63.77	В
	MOTA	178	CB	SER	36	64.347	-4.974	56.532	1.00 63.33	В
20	MOTA	179	og	SER	36	65.136	-4.438	55.481	1.00 61.84	В
20	ATOM	180	c	SER	36	62.240	-4.670	57.879	1.00 63.32	B
	MOTA	181	ŏ	SER	36	62.731	-5.313	58.810	1.00 63.79	В
		182			37					В.
	MOTA		N	ALA		60.939	-4.417	57.772	1.00 61.85	
25	MOTA	183	CA	ALA	37	59.989	-4.873	58.773	1.00 59.96	В
23	MOTA	184	СВ	ALA	37	58.921	-3.806	58.987	1.00 59.90	В
	MOTA	185	C	ALA	37	59.344	-6.219	58.442	1.00 58.87	В
	MOTA	186	0	ALA	37	58.975	-6.499	57.301	1.00 58.65	В
	MOTA	187	N	HIS	38 .	59.215	-7.038	59.479	1.00 57.20	В
30	MOTA	188	CA	HIS	38	58.638	-8.378	59.411	1.00 54.48	В
30	MOTA	189	CB	HIS	38	59.315	-9.263	60.513	1.00 56.18	В
	MOTA	190	CG	HIS	38	59.436	-8.582	61.851	1.00 56.74	B
	MOTA	191	CD2		38	59.058	-8.977	63.092	1.00 57.32	В
	ATOM	192	ND1		38	60.024	-7.344	62.011	1.00 55.67	В
25	MOTA	193	CE1		38	60.005	-7:006	63.288	1.00 56.12	В
35	MOTA	194	NE2		38	59.424	-7.980	63.967	1.00 57.53	В
	MOTA	195	C	HIS	38	57.118	-8.352	59.615	1.00 51.90	В
	MOTA	196	0	HIS	38	56.642	-8.343	60.754	1.00 52.05	В
	MOTA	197	N	SER	39	56.356	-8.350	58.523	1.00 47.82	В
40	MOTA	198	CA	SER	39	54.893	-8.320	58.619	1.00 44.47	В
40	MOTA	199	CB	SER	39	54.255	-8.336	57.219	1.00 43.58	В
	MOTA	200	OG	SER	39	52.837	-8.377	57.305	1.00 37.62	В
	MOTA	201	C	SER	39	54.303	-9.468	59.435	1.00 43.06	В
	MOTA	202	0	SER	39	54.681	-10.624	59.246	1.00 42.78	В
. ~	MOTA	203	N	ILE	40	53.373	-9.144	60.334	1.00 41.07	B
45	MOTA	204	CA	ILE	40	52.727	-10.162	61.157	1.00 39.33	В
	ATOM	205	CB	ILE	40	52.660	-9.761	62.665	1.00 39.17	В
	MOTA	206	CG2	ILE	40	54.063	-9.542	63.215	1.00 38.53	B
	ATOM	207	CGl	ILE	40	51.824	-8.511	62.858	1.00 39.67	В
	MOTA	208	CD1	ILE	40	51.496	-8.238	64.319	1.00 38.82	В
50	MOTA	209	С	ILE	40	51.314	-10.456	60.663	1.00 38.28	В
	MOTA	210	0	ILE	40	50.591	-11.249	61.265	1.00 37.83	В
	MOTA	211	N	VAL	41	50.932	-9.837	59.550	1.00 38.34	В
	MOTA	212	CA	VAL	41	49.597	-10.047	59.000	1.00 38.90	В
	MOTA	213	CB	VAL	41	48.792	-8.724	58.956	1.00 39.34	В
55	MOTA	214	CG1		41	47.421	-8.971	58.345	1.00 38.41	В
	MOTA	215	CG2		41	48.648	-8.154	60.360	1.00 38.28	В
	MOTA	216	С	VAL.	41		-10.683	57.612	1.00 38.55	В
	ATOM	217	Ó	VAL	41		-10.243	56.661	1.00 36.24	В
	MOTA	218	N	GLU	42		-11.729	57.513	1.00 40.08	В
60	MOTA	219		GLU	42		-12.433	56.255	1.00 42.70	В
••	ATOM	220		GLU	42		-13.916	56.393	1.00 45.52	В
	ATOM	221		GLU	42		-14.215	56.163	1.00 47.68	В
	ATOM	222		GLU	42		-15.636	56.578	1.00 50.75	B
	ATOM	223	OE1		42		-16.576	56.323	1.00 52.01	В
65	MOTA	224	OE2		42		-15.816	57.151	1.00 52.01	В
55	ATOM	225								
				GLU	42		-12.338	55.896	1.00 41.88	В
	MOTA	226		GLU	42		-12.740	56.683	1.00 42.51	В
	MOTA	227		CYS	43		-11.798	54.718	1.00 40.93	В
70	MOTA	228		CYS	43		-11.670	54.275	1.00 41.17	В
70	MOTA	229		CYS	43		-10.237	53.775	1.00 39.59	В
	MOTA	230		CYS	43	44.959	-9.008	55.115	1.00 41.44	В
	MOTA	231		CYS	43		-12.682	53.185	1.00 42.27	В
	MOTA	232	0	CYS	43	45.736	-12.781	52.182	1.00 43.23	В

	MOTA	233	N	ASP	44	43.953	-13.435	53.394	1.00 43.10	В
	ATOM	234		ASP	44		-14.444	52.436	1.00 43.06	В
	MOTA	235	CB	ASP	44	43.392	-15.831	53.138	1.00 45.99	В
-	MOTA	236		ASP	44		-16.999	52.151	1.00 46.99	В
5	MOTA	237	OD1		44		-16.948	51.139	1.00 48.57	В
	ATOM	238	OD2		44		-17.971	52.398	1.00 44.91	B B
	MOTA MOTA	239 240		ASP ASP	44		-14.045 -14.446	51.853 52.363	1.00 42.13	В
	MOTA	241		PRO	45		-13.254	50.767	1.00 41.84	В
10	ATOM	242		PRO	45		-12.853	49.990	1.00 40.65	В
	MOTA	243		PRO	45		-12.791	50.107	1.00 41.77	В
	ATOM	244		PRO	45		-12.001	48.918	1.00 41.50	8
	MOTA	245	CG	PRO	45	42.755	-12.688	48.614	1.00 40.93	В
. ~	ATOM	246	С	PRO	45	39.940	-13.893	49.690	1.00 42.90	В
15	MOTA	247		PRO	45		-13.822	50.002	1.00 43.83	В
	MOTA	248		VAL	46		-14.908	48.985	1.00 42.74	В
	HOTA	249		VAL	46		-15.990	48.552	1.00 42.50 1.00 41.92	B B
	MOTA MOTA	250 251	CB CG1	VAL	46 46		-17.109 -18.269	47.854 47.531	1.00 40.40	В
20	ATOM	252	CG2		46		-16.574	46.581	1.00 41.19	В
	ATOM	253		VAL	46		-16.577	49.751	1.00 43.26	В
	ATOM	254		VAL	46		-16.736	49.730	1.00 43.10	В
	ATOM	255	N	ARG	47	39.563	-16.896	50.797	1.00 43.54	В
0.5	MOTA	256	CA	ARG	47	38.975	-17.455	52.007	1.00 44.21	B
25	MOTA	257		ARG	47		-18.250	52.784	1.00 47.76	В
	ATOM	258		ARG	47		-19.635	52.203	1.00 52.08	В
	MOTA	259		ARG	47		-19.981	52.208 53.508	1.00 55.86 1.00 59.28	B B
	MOTA MOTA	260 261		ARG ARG	47 47		-19.743 -20.346	54.638	1.00 60.15	В
30	MOTA	262	NH1		47		-21.237	54.639	1.00 60.50	В
50	MOTA	263	NH2		47		-20.051	55.770	1.00 60.66	В
	ATOM	264		ARG	47		-16.360	52.883	1.00 41.71	В
	MOTA	265		ARG	47	37.673	-16.643	53.845	1.00 40.72	В
26	MOTA	266		LYS	48		-15.112	52.537	1.00 39.92	В
35	MOTA	267		LYS	48		-13.947	53.268	1.00 38.19	В
	MOTA	268		LYS	48		-13.912	53.223	1.00 38.15	В
	MOTA	269		LYS	48		-13.820 -14.236	51.826	1.00 39.40	B B
	MOTA MOTA	270 271		LYS	48 48		-14.236	51.809 50.440	1.00 39.31	В
40	MOTA	272		LYS	48		-14.620	49.354	1.00 42.78	В
••	ATOM	273		LYS	48		-13.925	54.723	1.00 37.09	В
	ATOM	274		LYS	48		-13:563	55.617	1.00 37.31	В
	MOTA	275	N	GLU	49	39.917	-14.314	54.961	1.00 35.98	В
4.5	MOTA	276		GLU	49		-14.327	56.315	1.00 36.33	В
45	ATOM	277		GLU	49		-15.733	56.743	1.00 40.35	В
	ATOM	278		GLU	49		-16.767	56.761	1.00 46.19	В
	ATOM	279		GLU	49 49		-18.163	57.122 56.975	1.00 49.22 1.00 50.87	B B
	MOTA MOTA	280 281	OE1 OE2		49		-19.131 -18.293	57.555	1.00 49.58	В
50	MOTA	282		GLU	49		-13.444	56.445	1.00 35.96	В
	MOTA	283		GLU	49		-13.095	55.462	1.00 34.28	B
	MOTA	284		VAL	50		-13.097	57.685	1.00 34.47	В
	MOTA	285	CA	VAL	50	43.122	-12.292	57.999	1.00 34.53	В
	MOTA	286		VAL	50		-10.858	58.439	1.00 32.83	В
55	ATOM	287	CG1		50		-10.918	59.512	1.00 30.31	В
	ATOM	288	CG2		50		-10.092	58.929	1.00 32.98	В
	MOTA	289		VAL	50		-13.059	59.135 60.130	1.00 35.60	B B
	ATOM ATOM	290 291		VAL SER	50 51		-13.367 -13.411	58.976	1.00 36.44	B
60	MOTA	292		SER	51		-14.157	60.022	1.00 36.92	В
00	ATOM	293		SER	51		-15.481	59.447	1.00 37.59	В
	MOTA	294		SER	51		-16.427	60.482	1.00 36.23	B
	ATOM	295		SER	51		-13.315	60.656	1.00 37.31	В
	ATOM	296		SER	51		-12.731	59.960	1.00 36.32	В
65	MOTA	297	N	VAL	52	46.852	-13.265	61.984	1.00 37.74	В
	MOTA	298	CA	VAL	52	47.817	-12.474	62.735	1.00 39.56	В
	MOTA	299		VAL	52		-11.558	63.749	1.00 38.44	В
	ATOM	300	CG1		52		-10.668	64.454	1.00 37.83	В
70	MOTA	301	CG2		52		-10.737	63.042	1.00 37.78	В
70	MOTA			VAL	52		-13.328	63.507	1.00 41.45	В
	ATOM	303		VAL	52 53		-14.296	64.167	1.00 41.94	B B
	MOTA MOTA	304 305		ARG ARG	53 53		-12.968 -13.713	63.434 64.166	1.00 45.18	B B
	21011	505	ų,			31.100		24.100	10.01	-

	MOTA	306	CB	ARG	53	52.452	-13.698	63.434	1.00 45.91	В
	ATOM	307	CG	ARG	53	53.488	-14.619	64.064	1.00 44.72	В
	MOTA	308	CD	ARG	53		-15.103		1.00 45.80	В
								63.034		
~	ATOM	309	NE	ARG	53		-14.018	62.514	1.00 46.75	В
5	MOTA	310	CZ	ARG	53	56.036	-14.095	61.398	1.00 45.30	В
	MOTA	311	NH1	ARG	53	56.028	-15.209	60.675	1.00 44.24	В
	ATOM	312		ARG	53		-13.056	61.011	1.00 44.19	В
	MOTA	313	С	ARG	53		-13.092	65.540	1.00 47.93	В
	ATOM	314	0	ARG	53	51.466	-11.884	65.667	1.00 48.40	В
10	ATOM	315	N	THR	54	51,156	-13.929	66.565	1.00 49.62	В
	MOTA	316	CA	THR	54		-13.473	67.941	1.00 51.39	В
	MOTA	317	CB	THR	54		-13.744	68.683	1.00 51.01	В
	ATOM	318	OG1	THR	54	49.735	-15.157	68.795	1.00 49.13	В
	MOTA	319	CG2	THR	54	48.775	-13.144	67.914	1.00 51.53	В
15	ATOM	320	С	THR	54	52.391	-14.139	68.709	1.00 52.60	В
		321			54	52.439				В
	ATOM		0	THR			-14.058	69.933	1.00 53.07	
	MOTA	322	N	GLY	55		-14.784	67.995	1.00 54.10	В
	MOTA	323	CA	GLY	55	54.404	-15.459	68.666	1.00 57.08	В
	ATOM	324	С	GLY	55	55.721	-15.519	67.914	1.00 59.62	В
20	ATOM	325	o	GLY	55	56.119		67.264	1.00 59.27	В
	MOTA	326	N	GLY	56		-16.668	68.016	1.00 60.97	В
	ATOM	327	CA	GLY	56	57.682	-16.880	67:372	1.00 62.99	В.
	MOTA	328	C	GLY	56	57.782	-16.549	65.892	1.00 64.76	В
	MOTA	329	0	GLY	56		-15.828	65.350	1.00 66.18	·B
25										
23	ATOM	330	N	LEU	57		-17.074	65.235	1.00 64.97	В
	MOTA	331	CA	LEU	57	59.032	-16.821	63.809	1.00 64.92	В
	MOTA	332	CB	LEU	57	60.508	-17.137	63.407	1.00 63.43	В
	ATOM	333	CG	LEU	57		-16.508	64.258	1.00 63.25	В
	ATOM	334		LEU	57		-17.335	65.520	1.00 62.77	В
30										
20	MOTA	335	CDZ	LEU	57		-16.452	63.459	1.00 61.76	В
	MOTA	336	С	LEU	57	58.080	-17.654	62.951	1.00 65.79	В
	ATOM	337	0	LEU	57	57.186	-18.328	63.470	1.00 65.88	В
	MOTA	338	N	ALA	58		-17.597	61.636	1.00 65.65	В
	MOTA			ALA			-18.356			
35		339	CA		58			60.712	1.00 65.12	В
22	MOTA	- 340	CB	ALA	58	57.687	-17.891	59.286	1.00 65.82	B
	ATOM	341	С	ALA	58	57.770	-19.838	60.847	1.00 64.20	В
	MOTA	342	0	ALA	58	56.953	-20.709	60.525	1.00 64.59	В
	ATOM	343	N	ASP	59		-20.099			В
								61.340	1.00 62.61	
40	MOTA	344	CA	ASP	59		-21.447	61.542	1.00 60.18	В
40	MOTA	345	СВ	ASP	59	60.973	-21.335	62.035	1.00 60.66	В
	ATOM	346	CG	ASP	59	61.622	-22.682	62.266	1.00 61.45	В
	ATOM	347	OD1	ASP	59		-23.268	63.343	1.00 61.95	В
	ATOM	348		ASP	59					
							-23.155	61.370	1.00 61.61	В
AE	MOTA	349	С	ASP	59		-22.274	62.519	1.00 58.06	В
45	MOTA	350	0	ASP	59	58.519	-23.490	62.370	1.00 56.73	В
	ATOM	351	N	LYS	60	58.109	-21.591	63.513	1.00 55.07	В
	MOTA	352	CA	LYS	60		-22.200	64.528	1.00 52.63	В
	MOTA	353	CB	LYS	60	58.107	-23.079	65.525	1.00 51.66	В
CO	MOTA	354	CG	LYS	60	57.301	-23.696	66.672	1.00 51.86	В
50	MOTA	355	CD	LYS	60	58.046	-24.839	67.368	1.00 51.88	В
	MOTA	356	CE	LYS	60	59.349	-24.373	68.011	1.00 53.18	В
	MOTA	357	NZ	LYS	60		-25.492	68.528	1.00 52.09	В
	MOTA	358	C	LYS	60 -		-21.023	65.248	1.00 51.19	В
	MOTA	359	0	LYS	60	57.314	-20.124	65.724	1.00 51.41	В
55	MOTA	360	N	SER	61	55.287	-21.010	65.313	1.00 48.55	В
	ATOM	361	CA	SER	61	54.599	-19.905	65.960	1.00 45.99	В
	ATOM	362	CB	SER	61		-18.636	65.192	1.00 46.32	В
	MOTA	363	OG	SER	61		-18.803	63.820	1.00 44.99	В
	MOTA	364	С	SER	61	53.092	-20.082	66.086	1.00 45.35	В
60	MOTA	365	0	SER	61	52:491	-20.950	65.449	1.00 44.81	В
	ATOM	366	N	SER	62		-19.242		1.00 43.72	R
							-19.261			_
	ATOM	367	CA	SER	62			67.131	1.00 41.95	В
	MOTA	368	CB	SER	62		-19.050	.68.592	1.00 41.39	В
	MOTA	369	OG	SER	62	51.608	-18.079	69.135	1.00 41.34	В
65	ATOM	370	С	SER	62		-18.143	66.291	1.00 40.85	В
	ATOM	371	0	SER	62		-17.229	65.872	1.00 39.19	В
	MOTA	372	N	ARG	63		-18.221	66.031	1.00 40.24	В
	MOTA	373	CA	ARG	63	48.461	-17.207	65.226	1.00 38.90	В
	ATOM	374	CB	ARG	63		-17.514	63.695	1.00 39.76	В
70										
, ,	MOTA	375	CG	ARG	63		-17.554	63.205	1.00 41.62	В
	MOTA	376	CD	ARG	63		-17.897	61.725	1.00 43.20	В
	MOTA	377	NE	ARG	63	49.763	-16.776	60.866	1.00 46.47	В
	MOTA	378	CZ	ARG	63		-15.711	60.626	1.00 46.07	В
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	MOTA	379	NHI	ARG	63	51.728	-15.613	61.178	1.00 47.55	В
	ATOM	380	NH2		63		-14.741	59.833	1.00 45.86	В
	MOTA	381	C	ARG	63		-17.131	65.558	1.00 37.75	В
	MOTA	382	0	ARG	63		-18.050	66.143	1.00 36.32	B
5	MOTA	383	N	LYS	64		-16.019	65.174	1.00 37.15	В
	ATOM	384	CA	LYS	64		-15.788	65.400	1.00 35.14	В
	MOTA	385	CB	LYS	64		-14.607	66.342	1.00 36.48	В
	ATOM	386	CG	LYS	64		-14.826	67.760	1.00 37.70	В
	ATOM	387	CD	LYS	64		-15.510	68.604	1.00 40.04	В
10	MOTA	388	CE	LYS	64		-15.408	70.087	1.00 40.04	В
	MOTA	389	NZ	LYS	64		-15.861	70.893	1.00 40.98	В
	ATOM	390	С	LYS	64		-15.467	64.041	1.00 33.82	В
	ATOM	391	0	LYS	64		-14.590	63.329	1.00 35.17	В
	MOTA	392	N	THR	65		-16.173	63.669	1.00 31.23	В
15	MOTA	393	CA	THR	65		-15.928	62.377	1.00 30.10	В
	MOTA	394	CB	THR	65	42.784	-17.141	61.438	1.00 32.25	В
	MOTA	395	· 0G1	THR	65	44.171	-17.498	61.357	1.00 32.66	В
	ATOM	396	CG2	THR	65	42.279	-16.799	60.028	1.00 33.40	В
20	MOTA	397	С	THR	65	41.133	-15.597	62.503	1.00 28.24	В
20	MOTA	398	0	THR	65	40.440	-16.116	63.382	1.00 28.59	В
	MOTA	399	N	TYR	66	40.648	-14.720	61.630	1.00 24.28	В
	MOTA	400	CA	TYR	66	39.244	-14.335	61.665	1.00 22.45	В
	MOTA	401	CB	TYR	66		-12.976	62.362	1.00 19.03	В
25	MOTA	402	CG	TYR	66		-12.804	63.674	1.00 16.05	В
25	MOTA	403	CD1		66		-12.594	63.697	1.00 11.74	В
	MOTA	404	CE1		66		-12.377	64.894	1.00 13.31	В
	ATOM	405	CD2		66		-12.802	64.891	1.00 15.60	В
	ATOM	406	CE2		66		-12.586	66.097	1.00 13.06	В
30	ATOM	407	CZ	TYR	66		-12.368	66.090	1.00 15.20	В
50	ATOM	408	ОН	TYR	66		-12.100	67.272	1.00 19.72	В
	MOTA	409	C	TYR	66		-14.241	60.271	1.00 22.39	В
	MOTA	410	0	TYR	66		-13.876	59.317	1.00 21.02	В
	ATOM	411	N	THR	67 67		-14.580	60.167	1.00 23.76	В
35	MOTA ATOM	412 413	CA CB	THR THR	67 67		-14.523 -15.754	58.900	1.00 25.75	В
55	ATOM	414	OG1		67 67			5B.699	1.00 24.72	В
	ATOM	415	CG2		67		-16.923	58.702	1.00 28.23	В
	MOTA	416	C	THR	67		-15.664 -13.291	57.376	1.00 24.97	В
	MOTA	417	ò	THR	67		-13.026	58.864 59.811	1.00 26.39 1.00 26.22	B B
40	ATOM	418	N	PHE	68		-12.538	57.775	1.00 26.22	В
	ATOM	419	CA	PHE	68		-11.342	57.565	1.00 27.23	В
	ATOM	420	СВ	PHE	68		-10.056	57.673	1.00 25.89	В
	ATOM	421	CC	PHE	68	36.634	-9.893	58.997	1.00 27.52	В
	ATOM	422	CD1		68		-10.485	59.230	1.00 26.70	₿.
45	ATOM	423	CD2		68	36.037	-9.161	60.023	1.00 26.12	В
	ATOM	424	CE1		68		-10.350	60.464	1.00 25.62	В
	MOTA	425	CE2		68	36.662	-9.025	61.258	1.00 25.03	В
	ATOM	426	CZ	PHE	68	37.894	-9.619	61.478	1.00 25.92	В
	MOTA	427	С	PHE	68		-11.434	56.171	1.00 27.19	B
50	MOTA	428	0	PHE	68		-12.206	55.328	1.00 27.43	В
	ATOM	429	N	ASP	69		-10.631	55.926	1.00 26.71	В
	MOTA	430	CA	ASP	69	32.805	-10.629	54.636	1.00 27.55	В
	MOTA	431	CB	ASP	69	31.660	-9.635	54.684	1.00 27.61	В
	MOTA	432		ASP	69	30.623	-10.019	55.735	1.00 28.58	В
55	ATOM	433	OD1		69	30.578	-9.403	56.831	1.00 27.66	В
	MOTA	434	OD2		69	29.865	-10.972	55.461	1.00 28.48	В
	MOTA	435		ASP	69	33.738	-10.366	53.458	1.00 27.41	В
	MOTA	436		ASP	69	33.455	-10.771	52.334	1.00 27.23	В
6 0	ATOM	437		MET	70	34.861	-9.710	53.732	1.00 28.30	В
60	MOTA	438	CA	MET	70	35.865	-9.396	52.717	1.00 28.88	В
	MOTA	439	CB	MET	70	35.424	-8.213	51.821	1.00 30.69	В
	ATOM	440		MET	70	34.283	-8.469	50.867	1.00 31.73	В
	MOTA	441		MET	70	33.894	-6.957	49.923	1.00 36.68	В
~ ~	MOTA	442		MET	70	32.083	-7.049	49.877	1.00 34.73	В
65	MOTA	443		MET	70	37.141	-8.983	53.433	1.00 28.83	В
	MOTA	444		MET	70	37.098	-8.480	54.553	1.00 29.82	В
	MOTA	445		VAL	71	38.274	-9.188	52.780	1.00 27.33	В
	MOTA	446		VAL	71	39.553	-8.812	53.349	1.00 26.23	В
70	MOTA	447		VAL	71		-10.021	54.003	1.00 27.99	В
70	MOTA	448	CG1		71		-10.381	55.319	1.00 28.32	· B
	MOTA	449	CG2		71		-11.219	53.076	1.00 28.60	В
	MOTA	450		VAL	71	40.398	-8.233	52.231	1.00 25.01	В.
	MOTA	451	0	VAL	71	40.363	-8.713	51.100	1.00 24.55	В

	ATOM	452	N	PHE	72	41.146	-7.191	52.571	1.00 24.93	В
	ATOM	453	CA	PHE	72	42.005	-6.475	51.645	1.00 24.43	В
	ATOM	454	CB	PHE	72	41.444	-5.076	51.392	1.00 23.95	В
_	MOTA	455	CG	PHE	72	40.024	-5.059	50.903	1.00 23.17	В
5	MOTA	456		PHE	72	39.722	-5.376	49.583	1.00 22.75	В
	MOTA	457		PHE	72	38.991	-4.680	51.754	1.00 23.31	В
	MOTA	458		PHE	72	38.414	-5.310	49.113	1.00 23.87	В
	ATOM	459		PHE	72	37.679	-4.612	51.294	1.00 23.71	B B
10	MOTA MOTA	460 461	CZ C	PHE	72 72	37.389 43.381	-4.927 -6.321	49.970 52.266	1.00 24.15	В
10	ATOM	462	ò	PHE	72	43.522	-5.683	53.312	1.00 26.80	8
	MOTA	463	N	GLY	73	44.394	-6.885	51.621	1.00 24.77	В
	MOTA	464	CA	GLY	73	45.741	-6.774	52.142	1.00 23.03	В
	MOTA	465	С	GLY	73	46.352	-5.450	51.743	1.00 26.33	В
15	MOTA	466	0	GLY	73	45.698	-4.594	51.141	1.00 26.76	В
	MOTA	467	N	ALA	74	47.626	-5.284	52.062	1.00 27.88	B
	MOTA	468	CA	ALA	74	48.335	-4.054	51.752	1.00 28.98	В
	MOTA	469	CB	ALA	74	49.690	-4.074	52.427	1.00 29.52	В
20	MOTA	470	c	ALA	74	48.505	-3.802	50.260	1.00 29.91	В
20	MOTA MOTA	471 472	И О	ALA SER	74 75	49.037 48.051	-2.773 -4.726	49.865 49.426	1.00 31.84	B B
	ATOM	473	CA	SER	75	48.209	-4.728	47.982	1.00 34.31	В.
	MOTA	474	CB	SER	75	48.382	-5.914	47.318	1.00 32.52	В.
	ATOM	475	0G	SER	75	49.088	-6.785	48.183	1.00 36.15	В
25	ATOM	476	С	SER	75	46.994	-3.858	47.395	1.00 34.29	В
	MOTA	477	0	SER	75	47.066	-3.236	46.327	1.00 34.53	В
	MOTA	478	N	THR	76	45.882	-3.963	48.111	1.00 32.69	В
	MOTA	479	CA	THR	76	44:635	-3.364	47.675	1.00 32.77	В
30	MOTA	480 481	CB	THR	76 76	43.530	-3.549	48.744	1.00 32.84	В
50	MOTA MOTA	482		THR	76 76	43.612 42.158	-4.863 -3.380	49.305 48.120	1.00 31.95 1.00 33.21	B B
	ATOM	483	C	THR	76	44.803	-1.870	47.403	1.00 31.46	. B
	ATOM	484	ŏ	THR	76	45.305	-1.134	48.251	1.00 32.33	В
~ ~	MOTA	485	N	LYS	77	44.394	-1.430	46.218	1.00 29.15	В
35	MOTA	· 486	CA	LYS	77	44.469	-0.015	45.875	1.00 27.33	В
	ATOM	487	CB	LYS	77	44.906	0.155	44.423	1.00 29.39	В
	ATOM.	488	CG	LYS	77	46.342	-0.341	44.187	1.00 32.84	В
	MOTA MOTA	489 490	CE	LYS	77 77	46.949 46.241	0.180 -0.349	42.884 41.627	1.00 36.59	B B
40	ATOM	491	NZ	LYS	77	44.818	0.106	41.501	1.00 38.31	В
	ATOM	492	c	LYS	77	43.096	0.625	46.134	1.00 25.52	В
	MOTA	493	0	LYS	77	42.127	-0.088	46.371	1.00 23.25	В
	MOTA	494	N	GLN	78	43.018	1.956	46.115	1.00 24.22	В
45	MOTA	495	CA	GLN	78	41.759	2.652	46.398	1.00 22.43	В
43	MOTA	496	CB	GLN	78	41.935	4.177	46.226	1.00 22.53	В
	MOTA MOTA	497 498	CD CD	GLN	78 78	43.014 42.603	4.799 4.953	47.088 48.539	1.00 21.23	B B
	ATOM	499		GLN	78	42.235	3.988	49.192	1.00 18.03	В
	MOTA	500	NE2		78	42.661	6.178	49.045	1.00 21.65	В
50	MOTA	501	C	GLN	78	40.624	2.177	45.504	1.00 22.10	В
	MOTA	502	0	CLN	78	39.533	1.839	45.986	1.00 20.46	В
	MOTA	503	N	ILE	79 .	40.898	2.153	44.203	1.00 21.56	В
	MOTA	504	CA	ILE	79 20	39.929	1.746	43.194	1.00 23.67	В
55	MOTA MOTA	505 506	CB CG2	ILE	79 79	40.590 41.716	1.749 0.732	41.774	1.00 23.18	B B
	MOTA	507	CG1		79	39.574	1.416	40.705	1.00 21.98	В
	MOTA	508	CD1		79	38.563	2.492	40.470	1.00 23.15	В
	MOTA	509	С	ILE	79	39.303	0.366	43.475	1.00 25.91	В-
~ 0	MOTA	510	0	ILE	79	38.142	0.120	43.122	1.00 26.57	В
60	MOTA	511	N	ASP	80	40.061	-0.527	44.107	1.00 24.45	В
	ATOM	512	CA	ASP	80	39.547	-1.857	44.416	1.00 25.05	В
	MOTA	513	CB	ASP	80	40.694	-2.832	44.721	1.00 25.59	В
	ATOM ATOM	514 515	CG	ASP	80	41.691	-2.928	43.588	1.00 26.46	B B
65	MOTA	516	OD1		80 80	41.248 42.912	-2.925 -3.016	42.414	1.00 26.20 1.00 27.35	В
-•	MOTA	517	C	ASP	80	38.612	-1.809	45.611	1.00 24.84	В
	ATOM	518	ŏ	ASP	80	37.638	-2.553	45.686	1.00 23.83	В
	MOTA	519	N	VAL	81	38.924	-0.934	46.556	1.00 25.12	В
70	MOTA	520	CA	VAL	81	38.102	-0.794	47.742	1.00 25.00	В
70	ATOM	521	CB	VAL	81	38.749	0.174	48.750	1.00 22.43	В
	ATOM	522	CG1		81	37.698	0.713	49.716	1.00 21.58	8
	MOTA MOTA	523 524	CG2 C	VAL	81 81	39.855 36.753	-0.555 -0.250	49.509 47.320	1.00 20.63 1.00 27.16	Ð B
	E T ON	244	-	AVP	01	20.723	-0.430		1.00 27.10	Þ

	MOTA	525	0	VAL	81	35.707	-0.746	47.747	1.00 27.22	В
	MOTA	526	N	TYR	82	36.792	0.769	46.464	1.00 27.98	В
	MOTA	527	CA	TYR	82	35.580	1.406	45.987	1.00 28.04	В
	MOTA	528	CB	TYR	82	35.922	2.661	45.125	1.00 27.34	В
5	MOTA	529	cc	TYR	82	34.681	3.366	44.637	1.00 26.71	B
-	MOTA				82				1.00 26.63	B
		530		TYR		34.262	3.252	43.315		
	MOTA	531	CEI	TYR	82	33.054	3.808	42.893	1.00 29.11	В
	MOTA	532		TYR	82	33.866	4.063	45.529	1.00 27.27	В
• •	MOTA	533	CE2	TYR	82	32.660	4.620	45.128	1.00 28.67	В
10	MOTA	534	CZ	TYR	82	32.257	4.488	43.809	1.00 30.95	₿
	MOTA	535	OH	TYR	82	31.047	5.021	43.418	1.00 34.58	В
	ATOM	536	C	TYR	82	34.705	0.454	45.183	1.00 29.38	В
	MOTA	537	ō	TYR	82	33.498	0.322	45.448	1.00 28.44	В
		53B		ARG	83	35.312		44.206	1.00 30.12	В
15	MOTA		N				-0.212			
13	MOTA	539	CA	ARG	83	34.569	-1.136	43.365	1.00 32.33	В
	MOTA	540	CB	ARG	83	35.475	-1.667	42.238	1.00 32.84	В
	MOTA	541	CG	ARG	83	35.814	-0.610	41.177	1.00 36.78	В
	MOTA	542	CD	ARG	83	36.995	-1.024	40.298	1.00 39.59	В
	MOTA	543	NE	ARG	83	36.692	-2.180	39.459	1.00 45.16	В
20	ATOM	544	CZ	ARG	83	36.158	-2.110	38.242	1.00 46.77	В
	ATOM	545	NH1	ARG	83	35.870	-0.930	37.706	1.00 47.42	В
	ATOM	546	NH2	ARG	83	35.897	-3.226	37.567	1.00 47.17	В
	MOTA	547	c	ARG	83	33.930	-2.291	44.142	1.00 32.86	В
25	MOTA	548	0	ARG	83	32.786	-2.658	43.866	1.00 34.02	В
23	MOTA	549	N	SER	84	34.648	-2.834	45.125	1.00 32.13	В
	MOTA	550	CA	SER	84	34.159	-3.959	45.933	1.00 30.95	Ð
	MOTA	551	CB	SER	84	35.347	-4.712	46.558	1.00 32.34	В
	MOTA	552	OG	SER	84	36.301	-5.060	45.568	1.00 37.12	В
	MOTA	553	С	SER	84	33.186	-3.593	47.046	1.00 29.09	В
30	MOTA	554	0	SER	84	32.151	-4.241	47.225	1.00 29.03	В
	MOTA	555	N	VAL	85	33.522	-2.570	47.815	1.00 27.74	В
	MOTA	556	CA	VAL	85	32.652	-2.176	48.911	1.00 27.01	В
	ATOM								1.00 25.48	
		557	CB	VAL	85	33.481	-1.800	50.165		В
25	MOTA	558		VAL	85	32.566	-1.623	51.354	1.00 24.98	В
35	MOTA	559		VAL	85	34.514	-2.865	50.448	1.00 26.13	В
	MOTA	560	С	VAL	85	31.684	-1.024	48.613	1.00 25.90	В
	MOTA	561	0	VAL	85	30.480	-1.167	48.779	1.00 24.94	В
	MOTA	562	N	VAL	86	32.205	0.106	48.152	1.00 26.94	В
	ATOM	563	CA	VAL	86	31.368	1.281	47.916	1.00 27.62	В
40	ATOM	564	CB	VAL	86	32.227	2.551	47.793	1.00 25.49	B
	ATOM	565		VAL	86	31.384	3.763	48.096	1.00 25.95	. B
	MOTA	566		VAL	86	33.418	2.480	48.722	1.00 24.40	В
	ATOM	567	C	VAL	86	30.395	1.267	46.736	1.00 28.91	В
15	ATOM	568	0	VAL	86	29.254	1.709	46.874	1.00 27.52	В
45	ATOM	569	N	CYS	87	30.835	0.773	45.583	1.00 30.20	В
	MOTA	570	CA	CYS	87	29.978	0.748	44.402	1.00 31.96	В
	MOTA	571	CB	CYS	87	30.692	0.026	43.257	1.00 35.17	В
	MOTA	572	SG	CYS	87	30.072	0.418	41.599	1.00 41.71	В
	MOTA	573	С	CYS	87	28.593	0.126	44.653	1.00 32.37	В
50	ATOM	574	0	CYS	87	27.571	0.682	44.234	1.00 31:48	В
	ATOM	575	N	PRO	88	28.538	-1.028	45.347	1.00 31.98	В
	ATOM	576	CD	PRO	88	29.675	-1.840	45.803	1.00 32.51	В
							-1.712			
	MOTA	577	CA	PRO	88	27.272		45.648	1.00 30.72	В
55	ATOM	578	CB	PRO	88	27.720	-3.024	46.269	1.00 31.27	В
55	ATOM	579	CG	PRO	88	29.104	-3.223	45.739	1.00 32.03	В
	MOTA	580	С	PRO	88	26.407	-0.907	46.617	1.00 30.37	В
	ATOM	581	0	PRO	88	25.179	-0.928	46.528	1.00 29.46	В
	MOTA	582	N	ILE	89	27.060	-0.214	47.549	1.00 28.89	В
	MOTA	583	CA	ILE	89	26.372	0.607	48.539	1.00 26.92	В
60	ATOM	584	CB	ILE	89	27.325	1.032	49.677	1.00 27.36	В
••		585			89		1.827	50.728	1.00 29.65	В
	ATOM			ILE		26.562				
	MOTA	586		ILE	89	27.949	-0.202	50.327	1.00 28.47	В
	MOTA	587		ILE	89	28.880	0.116	51.493	1.00 28.07	В.
65	MOTA	588	c	ILE	89	25.815	1.866	47.883	1.00 26.45	В
65	MOTA	589	0	ILE	89	24.733	2.329	48.236	1.00 25.57	В
	MOTA	590	N	LEU	90	26.551	2.416	46.922	1.00 26.88	В
	MOTA	591	CA	LEU	90	26.097	3.618	46.242	1.00 27.21	В
	MOTA	592	CB	LEU	90	27.185	4.167	45.305	1.00 26.30	В
	ATOM	593	CG	LEU	90	26.768	5.457	44.531	1.00 28.27	В
70									1.00 28.27	
, 0	MOTA	594		LEU	90	26.300	6.546	45.499		В
	MOTA	595		LEU	90	27.936	5.952	43.707	1.00 30.13	В
	MOTA	596	c	LEU	90	24.828	3.334	45.451	1.00 28.12	В
	MOTA	597	0	LEU	90	23.914	4.156	45.423	1.00 27.80	В

	MOTA	598	N	ASP	91	24.778	2.168	44.811	1.00 29.04	В
	MOTA	599	CA	ASP	91	23.615	1.782	44.029	1.00 29.68	В
	ATOM	600	CB	ASP	91	23.888	0.479	43.238	1.00 30.25	В
	ATOM	601	CG	ASP	91	24.715	0.717			
5								41.975	1.00 33.21	В
,	MOTA	602		ASP	91	24.655	1.836	41.417	1.00 33.99	В
	MOTA	603		ASP	91	25.409	-0.225	41.522	1.00 34.57	В
	MOTA	604	С	ASP	91	22.412	1.604	44.950	1.00 29.79	В
	MOTA	605	0	ASP	91	21.265	1.785	44.542	1.00 29.34	В
	ATOM	606	N	GLU	92	22.684	1.254	46.199	1.00 30.26	В
10	ATOM	607	CA	GLU	92	21.632	1.077	47.191	1.00 33.20	В
	MOTA	608	CB	GLU	92	22.240	0.434	48.455	1.00 37.58	В
	MOTA	609	cc	GLU	92	21.243	-0.021	49.519	1.00 45.34	₿.
	MOTA	610	CD	GLU	92	20.622	-1.378	49.215	1.00 49.33	В
• -	MOTA	611	OEl		92	19.996	-1.963	50.134	1.00 51.49	В
15	MOTA	612	OE2	GLU	92	20.760	-1.851	48.061	1.00 50.48	В
	MOTA	613	С	GLU	92	21.036	2.471	47.516	1.00 32.34	B
	ATOM	614	0	GLU	92	19.816	2.659	47.548	1.00 31.40	В
	MOTA	615	N	VAL	93	21.921	3.438	47.757	1.00 29.83	В
	ATOM	616	CA	VAL	93	21.532	4.813	48.060	1.00 27.09	В
20	ATOM	617	СВ	VAL	93	22.794	5.732	48.216	1.00 27.00	В
20		618	CG1							
	MOTA				93	22.362	7.185	48.503	1.00 23.70	В
	MOTA	619	CG2		93	23.720	5.189	49.320	1.00 24.02	В.
	MOTA	620	С	VAL	93	20.661	5.384	46.936	1.00 25.06	В
~~	MOTA	621	0	VAL	93	19.631	6.005	47.184	1.00 23.16	В
25	MOTA	622	N	ILE	94	21.090	5.173	45.700	1.00 23.81	В
	MOTA	623	CA	ILE	94	20.357	5.679	44.554	1.00 26.20	В
	MOTA	624	CB	ILE	94	21.196	5.496	43.268	1.00 24.09	В
	ATOM	625	CG2		94	20:398	5.871	42.040	1.00 22.58	В
	MOTA	626	CG1		94	22.436	6.394	43.367	1.00 23.30	В
30										
50	MOTA	627	CD1		94	23.378	6.288	42.211	1.00 25.19	В
	MOTA	628	C	ILE	94	18.964	5.057	44.417	1.00 28.52	В
	MOTA	629	0	ILE	94	18.101	5.606	43.742	1.00 30.41	В
	MOTA	630	N	MET	95	18.729	3.925	45.073	1.00 31.00	В
	MOTA	631	CA	MET	95	17.408	3.305	45.032	1.00 32.10	В
.35	MOTA	. 632	CB	MET	95	17.501	1.789	45.171	1.00 35.87	В
	ATOM	633	CG	MET	95	17.836	1.059	43.885	1.00 39.09	В
	ATOM	634		MET	95	17.725	-0.743	44.078	1.00 46.44	В
	ATOM	635		MET	95	19.451	-1.155	44.567	1.00 42.73	В
	MOTA	636		MET	95	16.514	3.857	46.140	1.00 31.79	В
40										
70	MOTA	637		MET	95	15.340	3.518	46.204	1.00 32.44	В
	MOTA	638		GLY	96	17.069	4.697	47.016	1.00 31.15	В
	MOTA	639		GLY	96	16.274	5.290	48.083	1.00 30.86	В
	ATOM	640		GLY	96	16.506	4.778	49.497	1.00 31.33	В
	ATOM	641	0	GLY	96	15.695	5.005	50.398	1.00 31.96	В
45	ATOM	642	N	TYR	97	17.617	4.085	49.700	1.00 31.69	В
	MOTA	643	CA	TYR	97	17.951	3.539	51.009	1.00 31.47	В
	MOTA	644		TYR	97	18.620	2.119	50.859	1.00 35.21	В
	MOTA	645		TYR	97	17.707	0.979	50.448	1.00 38.09	В
	ATOM	646	CD1		97	16.856	0.369	51.374	1.00 38.78	В
50										
50	MOTA	647	CE1		97	16.060	-0.716	51.017	1.00 39.92	В
	MOTA	648		TYR	97	17.733	0.476	49.146	1.00 38.17	В
	MOTA	649	CE2		97	16.938	-0.606	48.777	1.00 40.59	В
	MOTA	650	CZ	TYR	97	16.105	-1.197	49.717	1.00 42.01	В
	MOTA	651		TYR	97	15.314	-2.262	49.350	1.00 44.26	В
55	ATOM	652	С	TYR	97	18.944	4.465	51.699	1.00 29.27	. В
	HOTA	653	0	TYR	97	19.557	5.309	51.055	1.00 29.87	- в
	MOTA	654		ASN	98	19.089	4.308	53.008	1.00 26.93	В
	ATOM	655		ASN	98	20.061	5.081	53.768	1.00 27.11	В.
	ATOM	656		ASN	98	19.500	5.509	55.156	1.00 27.12	В
60										
oo	MOTA	657		ASN	98	18:435	6.579	55.048	1.00 27.28	В
	MOTA	658	OD1		98	18.553	7.506	54.245	1.00 30.11	В
	MOTA	659	ND2		98	17.394	6.465	55.860	1.00 26.60	В
	ATOM	660		ASN	98	21.243	4.141	.53.975	1.00 26.22	В
	MOTA	661	0	ASN	98	21.055	2.971	54.292	1.00 25.58	В
65	MOTA	662		CYS	99	22.457	4.634	53.775	1.00 25.47	B
	MOTA	663		CYS	99	23.629	3.791	53.977	1.00 25.10	В
	MOTA	664		CYS	99	24.206	3.357	52.654	1.00 26.81	B
	MOTA	665		CYS	99	23.084				
							2.317	51.714	1.00 26.81	В
70	MOTA	666		CYS	99	24.697	4.486	54.798	1.00 23.75	В
70	MOTA	667		CYS	99	24.804	5.712	54.804	1.00 25.67	В
	MOTA	668		THR	100	25.482	3.683	55.496	1.00 20.94	В
	MOTA	669	CA	THR	100	26.549	4.181	56.341	1.00 19.27	В
	MOTA	670	CB	THR	100	26.076	4.266	57.795	1.00 17.86	В

		(7)	001	m	100	24 002	E 100	62 025	1.00 16.90	В
	MOTA	671		THR	100	24.992	5.192	57.875		
	ATOM	672	CG2	THR	100	27.202	4.714	58.708	1.00 17.10	В
	ATOM	673	C	THR	100	27. 7 60	3.247	56.269	1.00 19.78	В
	ATOM	674	0	THR	100	27.615	2.013	56.297	1.00 19.41	В
5	ATOM	675	N	ILE	101	28.945	3.846	56.170	1.00 17.12	В
_	ATOM	676	CA	ILE	101	30.194	3.096	56.112	1.00 13.84	18
							3.273	54.770	1.00 11.63	В
	MOTA	677	СВ	ILE	101	30.923				
	ATOM	678		ILE	101	32.193	2.459	54.763	1.00 11.54	В
	ATOM	679	CG1	ILE	101	30.029	2.847	53.614	1.00 11.12	В
10	ATOM	680	CD1	ILE	101	30.610	3.205	52.240	1.00 8.60 ·	В
	ATOM	681	С	ILE	101	31.088	3.655	57.189	1.00 14.61	В
	MOTA	682	ō	ILE	101	31.434	4.828	57.158	1.00 16.06	В
				PHE	102		2.814	58.149	1.00 16.69	В
	MOTA	683	N			31.454				
15	MOTA	684	CA	PHE	102	32.336	3.214	59.246	1.00 15.45	В
15	MOTA	685	CB	PHE	102	31.957	2.509	60.517	1.00 15.38	В
	MOTA	686	CG	PHE	102	30.704	3.002	61.158	1.00 17.02	В
	MOTA	687	CD1	PHE	102	30.746	4.068	62.060	1.00 14.70	В
	MOTA	688		PHE	102	29.489	2.341	60.937	1.00 15.06	В
	MOTA	689		PHE	102	29.601	4.468	62.744	1.00 15.17	В
20										В
20	ATOM	690		PHE	102	28.336	2.732	61.614	1.00 16.46	
	MOTA	691	CZ	PHE	102	28.389	3.797	62.523	1.00 16.06	В
	MOTA	692	С	PHE	102	33.770	2.789	58.956	1.00 13.66	В
	MOTA	693	0	PHE	102	34.004	1.767	58.335	1.00 14.29	В
	ATOM	694	N	ALA	103	34.723	3.571	59.431	1.00 14.00	В
25	ATOM	695	CA	ALA	103	36.135	3.230	59.309	1.00 13.68	В
							4.316	58.595	1.00 12.73	В
	MOTA	696	CB	ALA	103	36.894				
	MOTA	697	C	ALA	103	36.579	3.142	60.771	1.00 14.68	В
	ATOM	698	0	ALA	103	36.560	4.144	61.491	1.00 12.81	В
	ATOM	699	N	TYR	104	36.943	1.939	61.211	1.00 14.23	В
30	MOTA	700	CA	TYR	104	37.369	1.722	62.588	1.00 13.28	В
	MOTA	701	CB	TYR	104	36.415	0.741	63.271	1.00 13.08	В
	MOTA	702	CG	TYR	104	36.704	0.496	64.740	1.00 9.23	В
										В
	ATOM	703		TYR	104	37.774	-0.304	65.139	1.00 10.77	
25	MOTA	704		TYR	104	38.050	-0.519	66.497	1.00 8.87	В
35	MOTA	705	CD2	TYR	104	35.916	1.072	65.728	1.00 7.28	В
	ATOM	706	CE2	TYR	104	36.180	0.861	67.085	1.00 6.26	В
	· ATOM	707	CZ	TYR	104	37.245	0.063	67.459	1.00 6.63	В
	MOTA	708	OH	TYR	104	37.492	-0.189	68.791	1.00 6.91	В
	MOTA	709	C.	TYR	104	38.791	1.191	62.660	1.00 14.55	В
40										
40	MOTA	710	0	TYR	104	39.192	0.344	61.866	1.00 17.36	В
	MOTA	711	N	GLY	105	39.553	1.688	63.622	1.00 15.00	В
	MOTA	712	CA	GLY	105	40.920	1.239	63.760	1.00 16.15	В
	ATOM	713	С	GLY	105	41.818	2.222	64.480	1.00 18.48	В
	ATOM	714	0	GLY	105	41.464	3.383	64.733	1.00 19.06	В
45	MOTA	715	N	GLN	106	42.996	1.726	64.818	1.00 18.69	В
	ATOM	716	CA	GLN	106	44.012	2.480	65.524	1.00 20.40	В
	MOTA	717	CB	GLN	106	45.109	1.510	65.958	1.00 20.92	В
	MOTA	718	CG	GLN	106	46.494	2.093	65.959	1.00 25.11	В
	MOTA	719	CD	GLN	106	47.546	1.104	66.424	1.00 27.12	В
50	ATOM	720	OE1	GLN	106	47.724	0.033	65.833	1.00 29.47	В
	ATOM	721	NE2	GLN	106	48.254	1.462	67.486	1.00 24.05	В
	ATOM	722	С	GLN	106	44.595	3.602	64.668	1.00 22.74	В
	ATOM	723	ŏ	GLN	106	44.733	3.442	63.447	1.00 22.56	В
55	ATOM	724	N	THR	107	44.924	4.733	65.312	1.00 22.64	В
55	ATOM	725	CA	THR	107	45.526	5.893	64.637	1.00 21.79	8
	MOTA	726	CB	THR	107	46.070	6.943	65.659	1.00 22.17	B
	MOTA	727	OG1	THR	107	45.014	7.404	66.510	1.00 22.36	В
	ATOM	728		THR	107	46.675	8.142	64.927	1.00 19.97	В
	ATOM	729	c	THR	107	46.720	5.430	63.788	1.00 21.90	В
60								64.288	1.00 20.99	В
00	MOTA	730	0	THR	107	47.605	4.752			
	MOTA	731	Ŋ	GLY	108	46.739	5.796	62.510	1.00 22.46	В
	MOTA	732	CA	GLY	108	47.836	5.394	61.652	1.00 21.62	В
	MOTA	733	С	GLY	108	47.664	4.088	60.882	1.00 22.90	В
	ATOM	734	0	GLY	108	48.653	3.547	60.376	1.00 24.07	В
65	ATOM	735	N	THR	109	46.436	3.572	60.786	1.00 22.29	В
	MOTA	736	CA		109	46.197	2.321	60.050	1.00 21.18	В
				THR						
	ATOM	737	CB	THR	109	45.408	1.259	60.884	1.00 21.26	В
	MOTA	738		THR	109	44.159	1.814	61.335	1.00 20.11	В
	MOTA	739	CG2	THR	109	46.250	0.777	62.071	1.00 19.60	В
70	MOTA	740	С	THR	109	45.439	2.523	58.754	1.00 19.58	В
	MOTA	741	0	THR	109	45.126	1.551	58.068	1.00 20.97	В
	ATOM	742	N	GLY	110	45.125	3.776	58.428	1.00 17.22	В
		743	CA				4.048		1.00 12.69	В
	MOTA	,43	CA	GLY	110	44.415	4.040	57.193	1.00 12.03	

	MOTA	744	С	GLY	110	42.943	4.424	57.232	1.00 12.29	В
	ATOM	745	0	GLY	110	42.288	4.365	56.193	1.00 14.37	В
	MOTA	746	N	LYS	111	42.398	4.795	58.386	1.00 11.41	В
_	MOTA	747	CA	LYS	111	40.983	5.198	58.432	1.00 12.47	В
5	MOTA	748	CB	LYS	111	40.540	5.653	59.898	1.00 13.24	B
	MOTA	749	CG	LYS	111	40.379	4.53B	60.934	1.00 10.82	В
	MOTA	7.50	CD	LYS	111	39.805	5.061	62.229	1.00 6.09	В
	ATOM	751	CE	LYS	111	40.691	6.142	62.813	1.00 10.33	В
	MOTA	752	NZ	LYS	111	42.130	5.748	63.038	1.00 9.60	В
10	MOTA	753	c	LYS	111	40.742	6.363	57.465	1.00 13.44	В
	ATOM	754	ŏ	LYS	111	39.870	6.295	56.587	1.00 14.48	В
	MOTA	755	N	THR	112	41.538	7.423	57.614	1.00 14.82	B
	MOTA	756	CA	THR	112	41.403	8.613	56.773	1.00 15.93	В
		757	CB	THR	112	42.140	9.793	57.417	1.00 15.93	В
15	MOTA MOTA	758	OG1	THR	112	41.538	10.066	58.694	1.00 14.63	В
13				THR	112	42.055	11.040	56.522	1.00 13.41	В
	MOTA	759	CG2		112	41.870	8.426	55.323	1.00 17.21	В
	ATOM	760	C	THR				54.385	1.00 16.82	В
	ATOM	761	0	THR	112	41.318	9.021			В
20	MOTA	762	N	PHE	113	42.887	7.595	55.142	1.00 17.40	
20	MOTA	763	CA	PHE	113	43.398	7.313	53.811	1.00 16.82	В
	MOTA	764	CB	PHE	113	44.654	6.389	53.889	1.00 16.02	В
	MOTA	765	CG	PHE	113	45.233	6.054	52.540	1.00 17.10	В.
	MOTA	766		PHE	113	46.126	6.918	51.920	1.00 18.15	В
25	MOTA	767		PHE	113	44.836	4.911	51.868	1.00 18.15	В
25	MOTA	768		PHE	113	46.614	6.654	50.652	1.00 19.37	В
	MOTA	769		PHE	113	45.317	4.632	50.588	1.00 20.77	В
	MOTA	770	cz	PHE	113	46.208	5.508	49.980	1.00 21.58	В
	ATOM	771	С	PHE	113	42.305	6.615	52.997	1.00 15.35	В
20	MOTA	772	0	PHE	113	42.125	.6.894	51.816	1.00 13.50	В
30	MOTA	773	N	THR	114	41.590	5.700	53.647	1.00 14.49	В
	MOTA	774	CA	THR	114	40.524	4.942	53.008	1.00 13.72	В
	MOTA	775	CB	THR	114	40.119	3.722	53.868	1.00 14.47	В
	ATOM	776	OG1	THR	114	41.228	2.834	53.980	1.00 13.50	В
	MOTA	777	CG2	THR	114	38.944	2:984	53.258	1.00 10.99	В
35	ATOM	. 778	С	THR	114	39.283	5.773	52.764	1.00 13.62	В
	MOTA	779	0	THR	114	38.733	5.758	51.674	1.00 14.61	B
	ATOM	780	N	MET	115	38.842	6.499	53.784	1.00 15.54	В
	MOTA	781	CA	MET	115	37.635	7.311	53.663	1.00 16.98	В
	MOTA	782	CB	MET	115	37.121	7.711	55.043	1.00 17.73	B
40	ATOM	783	CG	MET	115 ⁻	36.776	6.525	55.938	1.00 22.32	В
	MOTA	784	SD	MET	115	35.694	5.280	55.139	1.00 24.33	В
	MOTA	785	CE	MET	115	34.110	6.102	55.162	1.00 17.96	В
	ATOM	786	c	MET	115	37.772	8.556	52.809	1.00 16.94	В
	ATOM	787	ō	MET	115	36.824	8.956	52.140	1.00 17.35	В
45	MOTA	788	N	GLU	116	38.947	9.168	52.816	1.00 16.96	В
	ATOM	789	CA	GLU	116	39.139	10.391	52.040	1.00 17.40	В
	MOTA	790	СВ	GLU	116	39.564	11.563	52.988	1.00 17.75	В
	ATOM	791	CG	GLU	116	38.457	12.038	53.929	1.00 20.71	В
	ATOM	792	CD	GLU	116	38.980	12.893	55.070	1.00 22.10	В
50	MOTA	793		GLU	116	40.113	13.404	54.961	1.00 26.78	В
50	ATOM	794		GLU	116	38.260	13.064	56.074	1.00 22.44	, B
	ATOM	795	C	GLU	116	40.178	10.211	50.953	1.00 16.14	В
	ATOM	796	ŏ	GLU	116	39.925	10.474	49.783	1.00 12.66	В
	ATOM	797	N	GLY	117	41.357	9.768	51.360	1.00 16.93	В
55		798	CA	GLY	117	42.425	9.585	50.406	1.00 21.10	В
55	MOTA	799		GLY	117	43.424	10.723	50.439	1.00 22.08	В
	ATOM		C					51.248	1.00 21.52	В
	MOTA	800	0	GLY	117	43.321	11.640	-		В
	MOTA	801	N	GLU	118	44.390	10.661	49.536	1.00 24.00	
40	MOTA	802	CA	GLU	118	45.436	11.664	49.457	1.00 26.12	В
60	MOTA	803	СВ	GLU	118	46.712	11.116	50.134	1.00 27.39	В
	ATOM	804	CG	GLU	118	46.574	11.023	51.647	1.00 32.78	В
	MOTA	805	CD	GLU	118	47.603	10.111	52.316	1.00 37.03	В
	MOTA	806		GLU	118	48.799	10.149	51.938	1.00 36.38	В
C =	MOTA	807	OE2		118	47.208	9.369	53.246	1.00 39.57	В
65	MOTA	808	С	GLU	118	45.702	12.026	48.000	1.00 26.11	В
	MOTA	809	0	GLU	118	45.079	11.481	47.088	1.00 24.83	B
	MOTA	810	N	ARG	119	46.613	12.961	47.780	1.00 25.93	В
	MOTA	811	CA	ARG	119	46.922	13.355	46.423	1.00 26.49	В
~~	MOTA	812	CB	ARG	119	47.076	14.913	46.313	1.00 24.19	В
70	MOTA	813	CG	ARG	119	45.824	15.737	46.642	1.00 18.83	В
	ATOM	814	CD	ARG	119	44.579	15.206	45.965	1.00 15.06	В
	MOTA	815	NE	ARG	119	44.755	14.940	44.542	1.00 15.80	В
	MOTA	816	CZ	ARG	119	44.761	15.869	43.591	1.00 18.90	В

		017			330	44 601	12 142	43 010	1 00 20 61	В
	MOTA	817 818	NH1 NH2	ARG	119 119	44.601 44.910	17.142 15.528	43.910 42.314	1.00 20.61 1.00 17.87	В
	MOTA MOTA	819	C	ARG	119	48.207	12.682	45.967	1.00 29.08	В
	ATOM	820	ō	ARG	119	49.178	12.572	46.735	1.00 27.84	В
5	ATOM	821	N	SER	120	48.205	12.192	44.731	1.00 30.37	В
-	MOTA	822	CA	SER	120	49.417	11.597	44.203	1.00 32.15	В
	ATOM	823	CB	SER	120	49.190	11.014	42.825	1.00 33.55	В
	MOTA	824	OG	SER	120	48.380	9.854	42.897	1.00 34.65	В
• •	MOTA	825	С	SER	120	50.287	12.839	44.123	1.00 31.39	В
10	ATOM	826	0	SER	120	49.849	13.883	43.651	1.00 31.19	В
	MOTA	827	N	PRO	121	51.522	12.745	44.599	1.00 30.67	В
	MOTA	828	CD	PRO	121	52.207	11.494	44.965	1.00 31.67	В
	ATOM	829	CA	PRO	121	52.455	13.870	44.595 45.270	1.00 31.71	B B
15	ATOM	830 831	CB.	PRO PRO	121 121	53.674 53.658	13.288	44.783	1.00 32.88	В
13	MOTA MOTA	832	C	PRO	121	52.788	14.511	43.240	1.00 32.30	В
	ATOM		. 0	PRO	121	52.557	13.925	42.176	1.00 32.32	В
	ATOM	834	N	ASN	122	53.319	15.733	43.319	1.00 30.43	В
	ATOM	835	CA	ASN	122	53.753	16.529	42.175	1.00 30.58	В
20	MOTA	836	CB	ASN	122	54.974	15.864	41.515	1.00 30.83	В
	ATOM	837	CG	ASN	122	. 56.101	16.850	41.250	1.00 29.55	В
	MOTA	838	OD1		122	56.512	17.589	42.139	1.00 30.20	В
	MOTA	839	ND2		122	56.614	16.849	40.032	1.00 29.25	В
25	MOTA	840	C	ASN	122	52.708	16.838	41.107	1.00 30.96	В
23	ATOM	841	0	ASN	122	53.022	16.840	39.916 41.540	1.00 28.89 1.00 31.29	B B
	ATOM	842	N CA	GLU	123 123	51.479 50.380	17.121 17.435	40.630	1.00 31.29	В
	MOTA MOTA	843 844	CB	GLU	123	50.437	18.873	40.222	1.00 29.75	В
	ATOM	845	CG	GLU	123	50.311	19.825	41.382	1.00 31.53	В
30	ATOM	846	CD	GLU	123	50.030	21.243	40.942	1.00 34.00	В
• •	ATOM	847	OE1		123	50.896	21.842	40.255	1.00 32.81	В
	ATOM	848	0E2	GLU	123	48.937	21.753	41.288	1.00 35.74	В
	MOTA	849	С	GLU	123	50.396	16.558	39.393	1.00 32.07	₿.
25	MOTA	850	0	GLU	123	50.246	17.038	38.272	1.00 32.39	В
35	MOTA	851	N	GLU	124	50.576	15.261	39.620	1.00 33.92	В
	MOTA	852	CA	GLU	124	50.628	14.269	38.558	1.00 33.69	В
	ATOM	853	CB	GLU	124	51.235	12.998	39.111 38.184	1.00 35.39	B B
	MOTA MOTA	854 855	CD CD	GLU	124 124	51.234 51.966	11.798 10.613	38.801	1.00 42.18	В
40	ATOM	856	0E1		124	51.802	10.390	40.026	1.00 42.52	В
10	ATOM	857		GLU	124	52.698	9.906	38.067	1.00 42.46	В
	ATOM	858	c	GLU	124	49.252	13.994	37.958	1.00 33.48	B
	MOTA	859	0	GLU	124	49.149	13.665	36.778	1.00 33.85	В
	ATOM	860	N	TYR	125	48.196	14.141	38.758	1.00 32.64	В
45	MOTA	861	CA	TYR	125	46.841	13.895	38.267	1.00 33.52	В
	MOTA	862	CB	TYR	. 125	46.261	12.523	38.817	1.00 33.48	В
	ATOM	863	CG	TYR	125	47.109	11.290	38.613	1.00 35.23	В
	ATOM	864	CD1		125	47.951	10.826	39.624	1.00 35.75	В
50	MOTA	865	CE1		125	48.709 47.046	9.668 10.565	39.461 37.422	1.00 36.41	B B
50	ATOM ATOM	866 867	CD2	TYR	125 125	47.803	9.403	37.242	1.00 37.22	В
	MOTA	868	cz	TYR	125	48.630	8.962	38.268	1.00 38.72	В
	ATOM	869	ОН	TYR	125	49.369	7.811	38.108	1.00 40.27	В
	MOTA	870	c	TYR	125	45.851	14.985	38.677	1.00 33.79	В
55	MOTA	871	0	TYR	125	46.150	15.834	39.520	1.00 34.63	В
	MOTA	872	N	THR	126	44.669	14.949	38.063	1.00 33.04	В
	MOTA	873	CA	THR	126	43.588	15.858	38.420	1.00 31.85	В
	MOTA	874	CB	THR	126	42.562	16.061	37.286	1.00 31.42	В
60	MOTA	875	OG1		126	42.214	14.790	36.723	1.00 29.37	В
60	MOTA	876	CG5		126	43.114	16.996	36.216	1.00 30.94	В
	ATOM	877	C	THR	126	42.911	15.061	39.518	1.00 31.76	В
	ATOM	878	0	THR	126	43.023	13.836	39.552	1.00 31.47	В
	ATOM	879	N	TRP	127	42.197	15.738 15.053	40.401	1.00 31.44	B B
65	MOTA MOTA	880 881	CA CB	TRP	127 127	41.559 40.749	16.048	41.507 42.357	1.00 30.17	B
55	ATOM	882	CB	TRP TRP	127	39.474	16.455	41.718	1.00 25.01	В
	ATOM	883	CD2		127	38.207	15.796	41.846	1.00 24.45	В
	MOTA	B84	CE2		127	37.285	16.514	41.059	1.00 24.12	В
	ATOM	885	CE3		127	37.764	14.662	42.546	1.00 22.04	В
70	ATOM	886	CD1		127	39.278	17.507	40.885	1.00 23.64	В
	MOTA	887	NE1	TRP	127	37.966	17.553	40.483	1.00 24.14	В
	ATOM	888	CZ2		127	35.937	16.143	40.952	1.00 25.81	В
	MOTA	889	CZ3	TRP	127	36.427	14.285	42.441	1.00 24.07	В

										_
•	MOTA	890	CH2	TRP	127	35.526	15.026	41.647	1.00 26.19	В
	MOTA	891	С	TRP	127	40.664	13.883	41.099	1.00 30.31	В
	ATOM	892	0	TRP	127	40.635	12.859	41.784	1.00 31.25	В
•	MOTA	893	N	GLU	128	39.945	14.014	39.991	1.00 30.25	В
5	MOTA	894	CA	GLU.	128	39.036	12.943	39.575	1.00 29.93	В
	MOTA	895	CB	GLU	128	38.010	13.477	38.601	1.00 30.66	В
	ATOM	896	CG	GLU	128	38.597	14.116	37.360	1.00 32.82	В
				GLU	128	37.522	14.757	36.522	1.00 37.02	В
	MOTA	897	CD							
10	MOTA	898		GLU	128	36.740	15.558	37.085	1.00 37.94	В
10	MOTA	899	OE2	GLU	128	37.450	14.460	35.309	1.00 39.71	В
	MOTA	900	C	GLU	128	39.692	11.704	38.977	1.00 28.41	В
			ō	GLU	128	39.004	10.755	38.623	1.00 28.40	В
	ATOM	901								
	MOTA	902	N	GLU	129	41.012	11.716	38.853	1.00 27.73	В
	ATOM	903	CA	GLU	129	41.724	10.574	38.303	1.00 26.98	В
15	MOTA	904	CB	GLU	129	42.343	10.919	36.940	1.00 25.80	В
	ATOM	905	CG	GLU	129	41.317	11.144	35.841	1.00 28.03	В
									1.00 33.17	В
	MOTA	906	CD	GLU	129	41.954	11.422	34.487		
	MOTA	907	OE1	GŁU	129	41.201	11.654	33.510	1.00 35.80	В
	MOTA	908	OE2	GLU	129	43.206	11.411	34.389	1.00 33.91	В
20	ATOM	909	С	GLU	129	42.807	10.110	39.257	1.00 27.19	В
20					129		9.117	38.997	1.00 28.14	В
	MOTA	910	0	GLU		43.480				
	ATOM	911	N	ASP	130	42.966	10.814	40.372	1.00 27.13	В.
	MOTA	912	CA	ASP	130	43.995	10.445	41.336	1.00 28.16	В
	MOTA	913	CB	ASP	130	44.092	11.498	42.458	1.00 29.19	·B
25									1.00 31.28	B
23	MOTA	914	CG	ASP	130	45.484	11.577	43.061		
	MOTA	915		ASP	130	46.026	10.525	43.470	1.00 31.52	В
	MOTA	916	OD2	ASP	130	46.039	12.695	43.125	1.00 33.01	В
	MOTA	917	С	ASP	130	43:690	9.068	41.925	1.00 27.22	В
		918	ō	ASP	130	42.646	8.865	42.551	1.00 27.12	В
20	MOTA									
30	MOTA	919	N	PRO	131	44.590	8.093	41.704	1.00 26.27	В
	MOTA	920	CD	PRO	131	45.722	8.143	40.760	1.00 25.74	В
	MOTA	921	CA	PRO	131	44.404	6.733	42.217	1.00 25.42	В
	ATOM	922	CB	PRO	131	45.436	5.928	41.431	1.00 25.20	В
25.	MOTA	923	CG	PRO	131	46.516	6.926	41.15B	1.00 25.28	В
35 ·	MOTA	. 924	С	PRO	131	44.550	6.586	43.734	1.00 25.10	В
	MOTA	925	0	PRO	131	44.317	5.514	44.284	1.00 25.70	В
	ATOM	926	N	LEU	132	44.939	7.659	44.414	1.00 25.55	В
					132	45.061		45.870	1.00 24.12	В
	MOTA	927	CA	LEU			7.615			
40	ATOM	928	CB	LEU	132	46.335	8.393	46.358	1.00 23.33	В
40	ATOM	929	CC	LEU	132	47.750	7.835	45.985	1.00 24.01	В
	ATOM	930	CD1	LEU	132	48.853	8.699	46.613	1.00 21.35	В
	ATOM	931		LEU	132	47.875	6.394	46.474	1.00 25.49	В
	MOTA	932	С	LEU	132	43.794	8.216	46.497	1.00 23.99	В
	ATOM	933	0	LEU	132	43.694	8.338	47.728	1.00 24.50	В
45	ATOM	934	N	ALA	133	42.831	8.587	45.650	1.00 21.97	В
	ATOM	935	CA	ALA	133	41.566	9.155	46.129	1.00 23.50	В
					133		9.710	44.958	1.00 19.96	В
	MOTA	936	CB	ALA		40.738				
	MOTA	937	С	ALA	133	40.760	8.097	46.896	1.00 24.12	В
	MOTA	93B	Ο.	ALA	133	40.766	6.914	46.552	1.00 24.63	В
50	MOTA	939	N	GLY	134	40.060	8.546	47.931	1.00 25.21	В
	ATOM	940	CA	GLY	134	39.289	7.646	48.763	1.00 23.61	В
	ATOM	941	C	GLY	134	37.831	7.541	48.387	1.00 23.90	В
	ATOM	942	0	GLY	134	37.399	8.030	47.344	1.00 25.12	В
	MOTA	943	N	ILE	135	37.075	6.887	49.261	1.00 22.33	В
55	MOTA	944	CA	ILE	135	35.657	6.662	49.055	1.00 19.60	В
	MOTA	945	СВ	ILE	135	35.048	5.962	50.295	1.00 17.94	В
										В
	MOTA	946		ILE	135	33.513	5.984	50.232	1.00 15.17	
	MOTA	947	CG1	ILE	135	35.604	4.531	50.381	1.00 13.85	В
	ATOM	948	CD1	ILE	135	35.402	3.883	51.712	1.00 11.57	В
60 ·	MOTA	949	C	ILE	135	34.886	7.941	48.751	1.00 19.64	В
•										
	MOTA		0	ILE	135	34.130	7.995		1.00 17.27	В
	MOTA	951	N	ILE	136	35.090	8.971	49.566	1.00 19.64	В
	MOTA	952	CA	ILE	136	34.383	10.229	49.377	1.00 19.00	В
	ATOM	953		·ILE	136	34.758	11.219	50.486	1.00 18.34	В
65										В
0.5	MOTA	954		ILE	136	34.174	12.595	50.188	1.00 19.49	
	MOTA	955	CG1	ILE	136	34.226	10.669	51.838	1.00 18.91	В
	MOTA	956	CD1	ILE	136	34.680	11.447	53.086	1.00 18.92	В
	ATOM	957	c	ILE	136	34.552	10.867	47.991	1.00 17.37	В
70	MOTA	958	0	ILE	136	33.614	10.888	47.207	1.00 15.94	В
70	ATOM	959	N	PRO	137	35.742	11.382	47.662	1.00 16.74	В
	MOTA	960	CD	PRO	137	37.083	11.311	48.259	1.00 16.29	В
	MOTA	961	CA.	PRO	137	35.785	11.963	46.318	1.00 17.68	В
										В
	ATOM	962	СВ	PRO	137	37.263	12.305	46.132	1.00 14.17	ь

	MOTA	963	CG	PRO	137	37.966	11.351	47.037	1.00 16.06	В
	MOTA	964	С	PRO	137	35.229	11.025	45.232	1.00 20.66	В
	MOTA	965	0	PRO	137	34.408	11.434	44.406	1.00 22.43	В
_	ATOM	966	N	ARG	138	35.651	9.764	45.232	1.00 21.33	В
5	MOTA	967	CA	ARG	138	35.154	8.825	44.224	1.00 21.16	В
	ATOM	968	CB	ARG	138	35.768	7.428	44.436	1.00 19.87	В
	ATOM	969	CG	ARG	138	37.251	7.370	44.138	1.00 18.07	В
	ATOM-	970	CD	ARG	138	37.812	5.989	44.402	1.00 17.00	В
	ATOM								1.00 14.48	В
10		971	NE	ARG	138	39.264	6.019	44.408		В
10	MOTA	972	cz	ARG	138	40.016	5.909	43.327	1.00 16.26	
	MOTA	973	NH1	ARG	138	39.446	5.743	42.137	1.00 15.29	В
	ATOM	974	NH2	ARG	138	41.337	6.004	43.433	1.00 14.85	В
	MOTA	975	С	ARG	138	33.630	8.705	44.202	1.00 21.32	В
	ATOM	976	0	ARG	138	33.021	8.644	43.139	1.00 25.00	В
15	MOTA	977	N	THR	139	33.009	8.667	45.370	1.00 20.40	В
	ATOM	978	CA	THR	139	31.562	8.540	45.436	1.00 20.86	В
	ATOM	979	СВ	THR	139	31.081	8.385	46.895	1.00 20.11	В
	MOTA	980	0G1		139	31.770	7.293	47.512	1.00 21.18	В
	MOTA	981		THR	139	29.583	8.120	46.944	1.00 18.68	B
20										В
20	MOTA	982	C	THR	139	30.883	9.753	44.815	1.00 23.10	
	ATOM	983	0	THR	139	29.955	9.613	44.014	1.00 24.95	В
	MOTA	984	И	LEU	140	31.340	10.944	45.189	1.00 23.71	В
	ATOM	985	CA	LEU	140	30.762	12.175	44.659	1.00 23.38	В
	ATOM	986	CB	LEU	140	31.480	13.401	45.23B	1.00 21.47	B
25	MOTA	987	CG	LEU	140	31.211	13.560	46.733	1.00 21.91	В
	ATOM	988	CD1	LEU	140	32.120	14.621	47.305	1.00 21.37	В
	ATOM	989		LEU	140	29.740	13.883	46.966	1.00 18.69	В
	MOTA	990	C	LEU	140	30.859	12.184	43.154	1.00 23.10	В
	ATOM	991	ō	LEU	140	29.870	12.395	42.467	1.00 21.86	В
30	MOTA	992	N	HIS	141	32.058	11.948	42.645	1.00 24.02	В
50								41.207	1.00 27.46	В
	ATOM	993	CA	HIS	141	32.272	11.927			В
	MOTA	994	CB	HIS	141	33.741	11.616	40.908	1.00 27.50	
	MOTA	995	CG	HIS	141	34.101	11.718	39.457	1.00 30.18	В
25	ATOM	996		HIS	141	34.041	10.807	38.457	1.00 30.98	В
35	MOTA	997	ND1	HIS	141	34.614	12.869	38.896	1.00 30.79	В
	MOTA	998	CE1	HIS	141	34.859	12.662	37.615	1.00 29.68	В
	· ATOM	999	NE2	HIS	141	34.520	11.419	37.324	1.00 31.87	В
	MOTA	1000	С	HIS	141	31.372	10.885	40.517	1.00 28.79	В
	MOTA	1001	o	HIS	141	30.835	11.133	39.432	1.00 30.63	В
40	ATOM	1002	N	GLN	142	31.196	9.728	41.154	1.00 27.09	В
. •	ATOM	1003	CA	GLN	142	30.392	8.664	40.579	1.00 26.11	В
	ATOM	1004	CB	GLN	142	30.660	7.381	41.302	1.00 27.58	В
									1.00 29.72	В
	MOTA	1005	CC	GLN	142	31.938	6.733	40.855		В
45	ATOM	1006	CD	GLN	142	32.001	6.617	39.344	1.00 31.15	
43	ATOM	1007		GLN	142	31.181	5.929	38.729	1.00 32.85	В
	MOTA	1008		GLN	142	32.969	7.300	38.735	1.00 29.44	В
	MOTA	1009	С	GLN	142	28.894	8.913	40.514	1.00 25.79	В
	MOTA	1010	0	GLN	142	28.238	8.494	39.564	1.00 25.19	В
	MOTA	1011	N	ILE	143	28.351	9.583	41.523	1.00 24.49	В
50	MOTA	1012	CA	ILE	143	26.928	9.888	41.555	1.00 23.07	В
	ATOM	1013	CB	ILE	143	26.581	10.716	42.805	1.00 22.41	В
	ATOM	1014	CG2	ILE	143	25.174	11.285	42.690	1.00 24.89	В
	MOTA	1015		ILE	143	26.727	9.856	44.044	1.00 21.77	В
	MOTA	1016		ILE	143	26.477	10.599	45.339	1.00 21.34	В
55	MOTA	1017	c	ILE	143	26.492	10.664	40.308	1.00 23.84	В
<i>.</i>	MOTA	1018	ŏ		143	25.417	10.425	39.769	1.00 23.49	В
	MOTA	1019	N	PHE	144	27.334	11.593	39.860	1.00 25.75	. В
	MOTA	1020	CA	PHE	144	27.044	12.418	38.690	1.00 27.59	В
C 0	MOTA	1021	СВ	PHE	144	28.019	13.657	38.638	1.00 26.93	В
60	MOTA	1022	CG	PHE	144	27.734	14.694	39.688	1.00 27.63	В
	ATOM	1023	CD1	PHE	144	26.583	15.478	39.614	1.00 28.58	В
	MOTA	1024	CD2	PHE	144	28.577	14.845	40.785	1.00 27.80	В
	ATOM	1025		PHE	144	26.271	16.396	40.626	1.00 28.69	₿
	ATOM	1026		PHE	144	28.279	15.756	41.802	1.00 27.42	B.
65	ATOM	1027	CZ	PHE	144	27.121	16.532	41.723	1.00 29.86	В
	ATOM	1028	c	PHE	144	27.129	11.621	37.394	1.00 28.56	В
						26.425				
	MOTA	1029	0	PHE	144		11.918	36.423	1.00 27.83	В
	MOTA	1030	N	GLU	145	27.998	10.614	37.382	1.00 30.60	В
70	MOTA	1031	CA	GLU	145		9.757	36.209	1.00 32.75	В
70	ATOM	1032	СВ	GLU	145	29.433	8.889	36.357	1.00 35.85	. В
	MOTA	1033	CG	GLU	145	30.742	9.673	36.317	1.00 42.03	₿
	ATOM	1034	CD	GLU	145	31.201	9.977	34.898	1.00 46.55	B
	ATOM	1035	OE1	GLU	145	32.014	10.916	34.699	1.00 47.36	B

	MOTA	1036	OE2	GLU	145	30.748	9.262	33.976	1.00 49.72	В
	MOTA	1037	С	GLU	145	26.934	8.854	36.040	1.00 32.32	В
	MOTA	1038	0	GLU	145	26.319	8.812	34.974	1.00 32.21	B
	MOTA	1039	N	LYS	146	26.573	8.150	37.104	1.00 31.79	В
5									1.00 34.10	B
,	MOTA	1040	CA	LYS	146	25.443	7.235	37.066		
	MOTA	1041	CB	LYS	146	25.340	6.463	38.430	1.00 34.57	В
	MOTA	1042	CG	LYS	146	26.693	5.973	38.952	1.00 35.68	· В
	ATOM	1043	CD	LYS	146	26.597	4.862	39.994	1.00 34.50	В
	MOTA	1044	CE	LYS	146	26.566	3.486	39.327	1.00 35.54	В
10	ATOM	1045	NZ	LYS	146	27.115	2.405	40.204	1.00 33.09	В
10										В
	MOTA	1046	C	LYS	146	24.098	7.888	36.721	1.00 34.95	
	MOTA	1047	0	LYS	146	23.320	7.342	35.929	1.00 35.60	В
	MOTA	1048	N	LEU	147	23.831	9.057	37.298	1.00 34.40	В
	MOTA	1049	CA	LEU	147	22.574	9.762	37.061	1.00 33.66	В
15	MOTA	1050	CB	LEU	147	22.154	10.477	38.336	1.00 32.95	В
	ATOM	1051	CG	LEU	147	21.963	9.607	39.554	1.00 33.64	В
	ATOM	1052		LEU	147	21.682	10.474	40.775	1.00 34.40	В
	MOTA	1053		LEU	147	20.809	8.645	39.308	1.00 35.51	В
20	MOTA	1054	С	LEU	147	22.634	10.772	35.907	1.00 34.15	₿
20	MOTA	1055	0	LEU	147	21.724	11.576	35.728	1.00 32.96	В
	ATOM	1056	N	THR	143	23.698	10.719	35.115	1.00 35.64	В
	ATOM	1057	CA	THR	148	23.863	11.656	34.011	1.00 36.46	В
	ATOM	1058	CB	THR	148	25.138	11.332	33.198	1.00 35.78	B.
	MOTA	1059	0G1		148	25.492	12.468	32.409	1.00 36.67	·B
25										
25	MOTA	1060	CG2		148	24.914	10.150	32.274	1.00 36.63	В
	MOTA	1061	С	THR	148	22.659	11.770	33.057	1.00 37.44	В
	MOTA	1062	0	THR	148	22.313	12.878	32.639	1.00 37.93	В
	MOTA	1063	N	ASP	149	22:019	10.653	32.712	1.00 35.78	В
	MOTA	1064	CA	ASP	149	20.867	10.706	31.807	1.00 35.94	В
30	MOTA	1065	CB	ASP	149	21.337	11.004	30.322	1.00 34.77	В
	ATOM	1066	CG	ASP	149	22.404	10.027	29.827	1.00 36.65	В
	MOTA							30.467	1.00 35.17	В
		1067		ASP	149	22.605	8.965			
	MOTA	1068		ASP	149	23.032	10.321	28.784	1.00 35.41	В
25	MOTA	1069	С	ASP	149	19.966	9.460	31.824	1.00 36.15	В
35	MOTA	1070	0	ASP	149	19.568	8.947	30.769	1.00 32.78	В
	ATOM	1071	N	ASN	150	19.639	8.987	33.025	1.00 36.51	В
	ATOM	1072	CA	ASN	150	18.781	7.819	33.181	1.00 38.16	В
	MOTA	1073	CB	ASN	150	19.218	6.992	34.417	1.00 37.97	B
	MOTA	1074	CG	ASN	150	19.159	7.785	35.704	1.00 37.13	В
40								35.742	1.00 37.20	В
70	MOTA	1075		ASN	150	19.548	8.951			
	ATOM	1076		ASN	150	18.694	7.148	36.774	1.00 36.82	В
	MOTA	1077	¢	ASN	150	17.314	8.240	33.305	1.00 39.47	В
	MOTA	1078	0	ASN	150	16.419	7.397	33.433	1.00 39.49	В
	ATOM	1079	N	GLY	151	17.077	9.549	33.245	1.00 39.29	В
45	MOTA	1080	CA	GLY	151	15.725	10.063	33.343	1.00 39.01	В
	MOTA	1081	С	GLY	151	15.333	10.349	34.772	1.00 39.23	В
	ATOM	1082	ŏ	GLY	151	14.170	10.612	35.063	1.00 40.53	В
									1.00 40.25	В
	MOTA	1083	N	THR	152	16.307	10.285	35.670		
50	ATOM	1084	CA	THR	152	16.069	10.547	37.085	1.00 40.87	В
50	MOTA	1085	CB	THR	152	16.730	9.463	37.960	1.00 39.78	В
	MOTA	1086	0G1	THR	152	16.146	8.191	37.655	1.00 43.27	В
	MOTA	1087	CG2	THR	152	16.531	9.764	39.437	1.00 40.09	В
	MOTA	1088	С	THR	152	16.643	11.918	37.448	1.00 41.24	В
	ATOM	1089	ŏ	THR	152	17.860	12.120	37.434	1.00 42.84	B
55									1.00 40.50	В
"	MOTA	1090	N	GLU	153	15.753	12.856	37.754		
	MOTA	1091	CA	GLU	153	16.140	14.216	38.118	1.00 39.45	В
	ATOM	1092	CB	GLU	153	14.910	15.143	38.054	1.00 41.77	В
	MOTA	1093	CG	GLU	153	15.258	16.606	37.831	1.00 47.08	В
	MOTA	1094	CD	GLU	153	15.903	16.847	36.474	1.00 49.24	В
60 ·	MOTA	1095		GLU	153	16.559	17.901	36.313	1.00 49.10	В
	MOTA	1096	OE2		153	15.747	15.988	35.570	1.00 49.10	В
	MOTA	1097	Ç	GLU	153	16.697	14.170	39.538	1.00 36.82	В
	MOTA	1098	0	GLU	153	16.140	13.472	40.387	1.00 35.59	В
c=	ATOM	1099	N	PHE	154	17.770	14.919	39.807	1.00 33.77	В
65	MOTA	1100	CA	PHE	154	18.380	14.877	41.140	1.00 31.58	В
	ATOM	1101	CB	PHE	154	19.302	13.644	41.212	1.00 29.10	В
	ATOM	1102	CG	PHE	154	20.572	13.797	40.414	1.00 25.93	В
	MOTA	1103		PHE	154	21.763	14.165	41.038	1.00 25.72	В
70	MOTA	1104		PHE	154	20.573	13.597	39.037	1.00 23.66	В
70	ATOM	1105		PHE	154	22.941	14.328	40.297	1.00 26.03	В
	ATOM	1106	CE2	PHE	154	21.741	13.758	3B.294	1.00 25.52	В
	ATOM	1107	CZ	PHE	154	22.930	14.123	38.925	1.00 24.44	В
	MOTA	1108	С	PHE	154	19.183	16.093	41.627	1.00 29.93	В
			_							

			_							
	MOTA	1109	0	PHE	154	19.651	16.924	40.850	1.00 30.00	В
	MOTA	1110	N	SER	155	19.357	16.157	42.940	1.00 28.97	В
	MOTA	1111	CA	SER	155	20.140	17.212	43.572	1.00 28.90	В
	MOTA	1112	CB	SER	155	19.225	18.281	44.243	1.00 26.53	В
5	MOTA	1113	OG	SER	155	18.732	17.844	45.502	1.00 24.48	В
	ATOM	1114	С	SER	155	21.010	16.537	44.635	1.00 28.97	В
	MOTA	1115	ō	SER	155	20.588	15.569	45.279	1.00 28.86	В
	MOTA	1116	N	VAL	156	22.221	17.047	44.819	1.00 29.35	В
				VAL	156	23.135	16.483	45.803	1.00 29.64	В
10	MOTA	1117	CA			24.431	15.977	45.125	1.00 28.79	В
10	MOTA	1118	CB	VAL	156				1.00 29.92	В
	MOTA	1119	CG1		156	25.280	15.208	46.124		
	MOTA	1120		VAL	156	24.089	15.116	43.930	1.00 29.12	В
	ATOM	1121	С	VAL	156	23.516	17.517	46.863	1.00 29.76	В
	MOTA	1122	0	VAL	156	23.925	18.627	46.532	1.00 30.11	В
15	MOTA	1123	N	LYS	157	23.372	17.149	48.132	1.00 30.23	В
	ATOM	1124	CA	LYS	157	23.731	18.028	49.245	1.00 31.02	В
	MOTA	1125	CB	LYS	157	22.489	18.431	50.063	1.00 32.19	В
	ATOM	1126	CG	LYS	157	21.543	19.376	49.364	1.00 35.38	В
	MOTA	1127	CD	LYS	157	20.246	19.523	50.162	1.00 39.38	В
20	ATOM	1128	CE	LYS	157	19.169	20.259	49.369	1.00 39.91	В
	ATOM	1129	NZ	LYS	157	17.857	20.187	50.067	1.00 40.45	В
	ATOM .	1130	c	LYS	157	24.702	17.308	50.171	1.00 30.04	В
	ATOM	1131	ō	LYS	157	24.399	16.230	50.668	1.00 30.82	В
	ATOM	1132	N	VAL	158	25.866	17.900	50.402	1.00 27.97	В
25			CA		158	26.839	17.290	51.292	1.00 27.63	В
20	MOTA	1133		VAL		28.284	17.406	50.751	1.00 27.29	В
	MOTA	1134	CB	VAL	158				1.00 27.25	В
	MOTA	1135		VAL	158	28.433	16.582	49.478		В
	MOTA	1136		VAL	158	28.632	18.861	50.491	1.00 26.29	
20	MOTA	1137	C	VAL	158	26.785	17.959	52.649	1.00 27.62	В
30	MOTA	1138	0	VAL	158	26.182	19.009	52.818	1.00 27.51	В
	MOTA	1139	N	SER	159	27.431	17.344	53.624	1.00 28.77	В
	MOTA	1140	CA	SER	159	27.449	17.896	54.962	1.00 29.25	В
	MOTA	1141	CB	SER	159.	26.155	17.634	55.612	1.00 29.36	В
~ ~	MOTA	1142	OG	SER	159	26.083	18.324	56.835	1.00 35.64	В
35	MOTA	1143	С	SER	159	28.584	17.255	55.753	1.00 28.48	В
	ATOM	1144	0	SER	159	28.762	16.037	55.723	1.00 29.46	В
	ATOM	1145	N	LEU	160	29.364	18.070	56.451	1.00 26.66	В
	ATOM	1146	CA	LEU	160	30.473	17.529	57.215	1.00 26.24	В
	ATOM	1147	CB	LEU	160	31.769	18.008	56.649	1.00 26.22	В
40	ATOM	1148	CG	LEU	160	33.024	17.381	57.255	1.00 25.56	В
	ATOM	1149	CD1	LEU	160	32.850	15.873	57.350	1.00 24.56	В
	MOTA	1150	CD2	LEU	160	34.241	17.759	56.400	1.00 24.75	В
	MOTA	1151	С	LEU	160	30.393	17.872	58.690	1.00 26.51	В
	MOTA	1152	0	LEU	160	30.816	18.949	59.119	1.00 24.86	В
45	ATOM	1153	N	LEU	161	29.844	16.937	59.461	1.00 25.32	В
	ATOM	1154	CA	LEU	161	29.686	17.112	60.895	1.00 23.81	В
	ATOM	1155	CB	LEU	161	28.349	16.607	61.310	1.00 23.24	В
	ATOM	1156	CG	LEU	161	28.109	16.490	62.766	1.00 23.19	В
	ATOM	1157		LEU	161	27.992	17.879	63.371	1.00 24.82	В
50	ATOM	1158		LEU	161	26.838	15.701	62.989	1.00 22.84	B
50		1159	C	LEU	161	30.777	16.338	61.613	1.00 24.19	В
	MOTA						15.178	61.307	1.00 25.43	В
	MOTA	1160	0	LEU	161	31.024			1.00 23.45	В
	MOTA	1161	N	GLU	162	31.444	16.983	62.563		В
55	MOTA	1162	CA	GLU	162	32.507	16.322	63.304	1.00 21.29	
55	MOTA	1163	CB	GLU	162	33.892	16.895	62.872	1.00 19.65	B
	MOTA	1164	CG	GLU	162	34.027	16.956	61.338	1.00 18.31	В
	MOTA	1165	CD	GLU	162	35.463	16.923	60.845	1.00 19.90	В
	MOTA	1166	0E1	GLU	162	36.362	17.416	61.557	1.00 20.88	В
	MOTA	1167	OE2	GLU	162	35.699	16.413	59.729	1.00 21.08	В
60	ATOM	1168	C	GLU	162	32.276	16.448	64.803	1.00 21.51	В
	MOTA	1169	0	GLU	162	31.734	17.441	65.286	1.00 24.11	В
	MOTA	1170	N	ILE	163	32.665	15.419	65.543	1.00 20.50	В
	ATOM	1171	CA	ILE	163	32.464	15.414	66.979	1.00 16.52	В
	MOTA	1172	СВ	ILE	163	31.587	14.221	67.396	1.00 15.68	В
65	ATOM	1173		ILE	163	31.070	14.412	68.813	1.00 13.11	B
	ATOM	1174		ILE	163	30.420	14.093	66.427	1.00 14.88	В
				ILE	163	29.521	12.920	66.704	1.00 16.15	В
	MOTA	1175							1.00 17.43	В
	MOTA	1176	C	ILE	163	33.805	15.325	67.672		
70	MOTA	1177	0	ILE	163	34.644	14.499	67.319	1.00 17.59	В
70	MOTA	1178	N	TYR	164	33.996	16.201	68.654	1.00 17.46	В
	ATOM	1179	CA	TYR	164	35.219	16.263	69.430	1.00 16.57	В
	ATOM	1180	CB	TYR	164	36.192	17.276	68.783	1.00 14.70	В
	ATOM	1181	CC	TYR	164	37.464	17.474	69.559	1.00 12.25	В

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	MOTA	1182	CD1	TYR	164	37.502	18.334	70.653	1.00 13.17	В
	MOTA	1183		TYR	164	38.643	18.439	71.454	1.00 15.94	В
	MOTA	1184		TYR	164	38.600	16.724	69.267	1.00 13.00	В
5	MOTA	1185		TYR	164	39.753	16.814	70.058	1.00 15.22	В
ر	MOTA	1186 1187	CZ OH	TYR TYR	164 164	39.773 40.909	17.674 17.774	71.155 71.952	1.00 17.31 1.00 15.71	8 B
	MOTA MOTA	1188	C	TYR	164	34.875	16.669	70.863	1.00 18.56	В
	ATOM	1189	ŏ	TYR	164	34.289	17.726	71.094	1.00 21.94	В
	ATOM	1190	N	ASN	165	35.225	15.826	71.828	1.00 20.33	В
10	MOTA	1191	CA	ASN	165	34.942	16.122	73.232	1.00 22.94	В
	MOTA	1192	CB	ASN	165	35.633	17.402	73.653	1.00 24.28	В
	MOTA	1193	CC	ASN	165	36.418	17.255	74.942	1.00 28.53	В
	ATOM	1194		ASN	165	37.598	16.864	74.929	1.00 31.28	В
15	MOTA	1195 1196	C C	asn asn	165 165	35.777 33.443	17.569 16.314	76.064 73.406	1.00 24.86 1.00 24.90	B B
13	MOTA MOTA	1197	ō	ASN	165	33.009	17.222	74.121	1.00 26.77	В
	MOTA	1198	N	GLU	166	32.657	15.471	72.745	1.00 23.40	B
	MOTA	1199	CA	GLU	166	31.200	15.555	72.813	1.00 22.69	В
	MOTA	1200	CB	GLU	166	30.706	15.231	74.237	1.00 22.07	В
20	MOTA	1201	CG	GLU	166	30.814	13.757	74.590	1.00 22.71	В
	MOTA	1202	CD	GLU	166	30.157	12.849	73.548	1.00 23.19	В
	MOTA	1203	OE2	GLU	166 166	28.906	12.779 12.211	73.505 72.769	1.00 22.44 1.00 21.71	B. B
	MOTA MOTA	1204 1205	C	GLU	166	30.899 30.610	16.884	72.769	1.00 22.21	В
25	ATOM	1206	ŏ	CLU	166	29.491	17.228	72.709	1.00 22.53	В
_	MOTA	1207	N	GLU	167	31.363	17.631	71.545	1.00 24.18	B
	MOTA	1208	CA	GLU	167	30.885	18.899	71.011	1.00 23.58	В
	ATOM	1209	CB	GLU	167	31.825	20.009	71.365	1.00 28.43	B
30	ATOM	1210	CC	GLU	167	31.900	20.321	72.848	1.00 34.21	В
30	ATOM	1211 1212	CD	GLU	167 167	32.857 34.033	21.470 21.400	73.142 72.702	1.00 40.07 1.00 41.07	B B
	MOTA MOTA	1212		GLU	167	32.431	22.441	73.812	1.00 43.47	В
	ATOM	1214	.C	GLU	167	30.800	18.766	69.500	1.00 22.74	В
·	ATOM	1215	Ó	GLU	167	31.659	18.142	68.884	1.00 23.08	В
35	ATOM	1216	N	LEU	168	29.766	19.347	68.904	1.00 21.20	В
•	ATOM	1217	CA	LEU	168	29.578	19.274	67.461	1.00 20.52	В
	MOTA	1218	CB	LEU	168	28.088	19.156	67.125	1.00 21.09	В
	MOTA MOTA	1219 1220	CG	LEU	168 168	27.319 28.249	17.889	67.681 67.622	1.00 22.11 1.00 15.69	B B
40	ATOM	1221		LEU	168	26.837	18.136	69.114	1.00 21.13	В
	ATOM	1222	c	LEU	168	30.173	20.458	66.702	1.00 21.77	В
	ATOM	1223	0	LEU	168	30.178	21.598	67.179	1.00 22.45	В
	MOTA	1224	N	PHE	169	30.673	20.171	65.506	1.00 20.28	В
45	MOTA	1225	CA	PHE	169	31.282	21.180	64.665	1.00 19.17	В
43	ATOM ATOM	1226 1227	CB	PHE	169 169	32.835 33.345	21.112 21.308	64.778 66.177	1.00 19.31 1.00 19.18	B B
	MOTA	1228		PHE	169	33.688	20.213	66.966	1.00 20.05	В
	ATOM	1229		PHE	169	33.434	22.591	66.722	1.00 18.70	В
	MOTA	1230	CE1	PHE	169	34.112	20.385	68.281	1.00 19.61	В
50	MOTA	1231		PHE	169	33.852	22.782	68.027	1.00 18.44	В
	MOTA	1232	CZ	PHE	169	34.193	21.676	68.814	1.00 22.70	В
	MOTA MOTA	1233 1234	0	PHE	169 169	30.865 30.476	20.981 19.880	63.220 62.808	1.00 20.25 1.00 20.20	B B
	MOTA	1235	И	ASP	170	30.949	22.064	62.462	1.00 19.31	В
55	ATOM	1236	CA	ASP	170	30.603	22.069	61.053	1.00 19.06	В
	MOTA	1237	СВ	ASP	170	29.549	23.141	60.785	1.00 19.49	В
	ATOM	1238	ÇG	ASP	170	28.970	23.066	59.386	1.00 21.37	В
	MOTA	1239		ASP	170	29.648	22.556	58.463	1.00 20.46	В
60	ATOM	1240		ASP	170	27.827	23.542	59.206	1.00 24.10	В
w	MOTA MOTA	1241 1242	0	ASP ASP	170 170	31.902 32.402	22.429 23.540	60.353 60.509	1.00 20.21 1.00 21.52	B B
	ATOM	1243	N	LEU	171	32.460	21.492	59.599	1.00 20.15	В
	MOTA	1244	CA	LEU	171	33.699	21.758	.58.900	1.00 22.53	В
	ATOM	1245	CB	LEU	171	34.620	20.517	58.965	1.00 19.76	В
65	ATOM	1246	CG	LEU	171	35.385	20.297	60.340	1.00 18.93	В
	MOTA	1247		LEU	171	36.562	21.251	60.487	1.00 16.80	В
	MOTA	1248		LEU	171	34.426	20.479	61.495	1.00 18.41	В
	MOTA	1249	C	LEU	171	33.460	22.198	57.459	1.00 24.95	B B
70	MOTA MOTA	1250 1251	O N	LEU	171 172	34.374 32.233	22.169 22.618	56.632 57.160	1.00 25.06 1.00 28.25	В
. •	ATOM	1252	CA	LEU	172	31.910	23.081	55.812	1.00 23.25	В
	ATOM	1253	СВ	LEU	172	31.001	22.111	55.116	1.00 33.77	В
	MOTA	1254	CG	LEU	172	31.664	20.867	54.556	1.00 34.20	В

	MOTA	1255	CD1	LEU	172	30.632	20.056	53.783	1.00 33.48	В
	MOTA	1256		LEU	172	32.807	21.268	53.644	1.00 34.44	В
	ATOM	1257	c	LEU	172	31.279	24.461	55.766	1.00 35.97	В
									1.00 37.85	
5	MOTA	1258	0	LEU	172	31.181	25.059	54.706		В
5	MOTA	1259	N	ASN	173	30.843	24.962	56.912	1.00 39.07	В
	MOTA	1260	CA	ASN	173	30.242	26.284	56.972	1.00 44.33	В
	MOTA	1261	CB	ASN	173	29.451	26.445	58.275	1.00 45.10	В
	ATOM	1262	CG	ASN	173	28.700	27.765	58.345	1.00 47.21	В
	MOTA	1263		ASN	173	27.898	27.987	59.254	1.00 46.55	B
10										
10	MOTA	1264		ASN	173	28.958	28.650	57.384	1.00 47.66	В
	MOTA	1265	С	asn	173	31.355	27.330	56.903	1.00 48.18	В
	MOTA	1266	0	ASN	173	32.094	27.532	57.871	1.00 47.58	В
	MOTA	1267	N	PRO	174	31.492	28.007	55.752	1.00 51.96	В
	MOTA	1268	CD	PRO	174	30.737	27.802	54.502	1.00 52.92	В
15	MOTA	1269	CA	PRO	174	32.527	29.030	55.572	1.00 55.50	В
	MOTA	1270	СВ	PRO	174	32.609	29.162	54.076	1.00 54.73	В
	MOTA	1271	CC	PRO	174	31.184	28.973	53.660	1.00 53.60	В
	ATOM	1272	С	PRO	174	32.226	30.364	56.259	1.00 58.47	В
00	ATOM	1273	0	PRO	174	33:076	31.256	56.286	1.00 59.03	В
20	ATOM	1274	N	SER	175	31.024	30.497	56.819	1.00 60.76	В
	MOTA	1275	CA	SER	175	30.639	31.730	57.504	1.00 62.73	В
	MOTA .	1276	СВ	SER	175	29.138	32.013	57.301	1.00 63.76	В
	MOTA	1277	OG	SER	175	28.877	32.450	55.975	1.00 66.00	В
25	MOTA	1278	C	SER	175	30.957	31.725	59.000	1.00 63.50	В
23	MOTA	1279	0	SER	175	30.901	32.769	59.654	1.00 63.94	В
	MOTA	1280	N	SER	176	31.293	30.557	59.543	1.00 63.63	В
	MOTA	1281	CX	SER	176	31.613	30.456	60.964	1.00 63.17	В
	MOTA	1282	CB	SER	176	30.589	29.549	61.694	1.00 63.04	В
	ATOM	1283	OG	SER	176	30.805	28.181	61.389	1.00 64.15	В
30	MOTA	1284	c	SER	176	33.017	29.909	61.188	1.00 62.90	В
	ATOM	1285	ŏ	SER	176			60.238		В
						33.758	29.643		1.00 62.07	
	MOTA	1286	N	ASP	177	33.371	29.744	62.459	1.00 62.85	В
	MOTA	1287	CA	ASP	177	34.676	29.225	62.837	1.00 62.62	В
26	MOTA	1288	CB	ASP	177	35.352	30.147	63.856	1.00 63.20	В
35	MOTA	1289	CG	ASP	177	35.504	31.559	63.345	1.00 63.21	В
	ATOM	1290	OD1	ASP	177	36.062	31.729	62.243	1.00 63.09	В
	ATOM	1291		ASP	177	35.068	32.498	64.044	1.00 62.91	В
	MOTA	1292	C	ASP	177	34.515			1.00 61.87	В
							27.852	63.452		
40	MOTA	1293	0	ASP	177	33.447	27.504	63.954	1.00.62.79	B
40	MOTA	1294	N	VAL	178	35.588	27.078	63.415	1.00 60.45	В
	ATOM	1295	CA	VAL	178	35.572	25.743	63.977	1.00 59.51	В
	MOTA	1296	CB	VAL	178	36.894	25.005	63.688	1.00 59.52	В
	ATOM	1297	CG1	VAL	178	37.118	24.909	62.183	1.00 59.92	В
	ATOM	1298		VAL	178	38.048	25.729	64.356	1.00 59.97	В
45	ATOM	1299	c	VAL	178	35.363	25.834	65.485	1.00 58.12	В
	ATOM	1300	ò	VAL	178					В
						35.159	24.825	66.157	1.00 59.80	
	MOTA	1301	N	SER	179	35.421	27.047	66.016	1.00 55.31	В
	MOTA	1302	CA	SER	179	35.221	27.245	67.443	1.00 52.98	В
	ATOM	1303	СB	SER	179	35.823	28.578	67.871	1.00 51.75	В
50	ATOM	1304	OG	SER	179	35.401	29.619	67.011	1.00 50.71	В
	ATOM	1305	С	SER	179	33.725	27.211	67.746	1.00 52.04	В
	MOTA	1306	0	SER	179	33.313	26.894	68.860	1.00 52.07	В
	ATOM	1307	N	GLU	180	32.917	27.535	66.743	1.00 51.08	В
		1308	CA							
55	ATOM			GLU	180	31.467	27.541	66.882	1.00 50.67	В
23	MOTA	1309	СВ	GLU	180	30.834	28.188	65.639	1.00 53.74	В
	MOTA	1310	CG	GLU	180	29.322	28.334	65.691	1.00 57.88	В
	MOTA	1311	CD	GLU	180	28.872	29.401	66.666	1.00 60.00	В
	MOTA	1312	OE1	GLU	180	29.192	29.279	67.868	1.00 61.89	В
	ATOM	1313	OE2		180	28.199	30.362	66.230	1.00 61.08	В
60	ATOM	1314	c	GLU	180	30.989	26.096	67.026	1.00 48.91	В
00										_
	MOTA	1315	0	GLU	180	31.307	25.249	66.196	1.00 49.20	В
	ATOM	1316	N	ARG	181	30.234	25.817	68.082	1.00 46.31	8
	MOTA	1317	CA	ARG	181	29.739	24.472	68.332	1.00 44.31	В
	ATOM	1318	CB	ARG	181	30.194	24.01B	69.710	1.00 46.69	В
65	ATOM	1319	CG	ARG	181	29.815	24.962	70.842	1.00 50.74	В
	ATOM	1320	CD	ARG	181	28.527	24.530	71.547	1.00 55.78	B
	ATOM	1321	NE	ARG					1.00 60.23	
					181	28.677	23.242	72.234		В
	ATOM	1322	CZ	ARG	181	27.708	22.628	72.913	1.00 61.32	В
70	ATOM	1323	NH1		181	26.501	23.180	73.007	1.00 61.66	В
70	MOTA	1324	NH2	ARG	181	27.945	21.453	73.490	1.00 61.67	В
	MOTA	1325	С	ARG	181	28.217	24.395	68.211	1.00 42.65	В
	MOTA	1326	Ó	ARG	181	27.491	25.115	68.888	1.00 42.59	В
	ATOM	1327	N	LEU	182	27.739	23.510	67.344	1.00 39.35	В
			••		202	27.733	23.310	JJ44	2.00 33.33	-

	MOTA	1328	CA	LEU	182	26.310	23.355	67.110	1.00 35.22	В
	MOTA	1329	CB	LEU	182	26.088	22.559	65.843	1.00 32.83	В
	MOTA	1330	CG	LEU	182	26.998	22.979	64.710	1.00 31.23	В
	ATOM	1331		LEU	182	26.730	22.114	63.508	1.00 32.55	В
5	ATOM	1332		LEU	182	26.776	24.444	64.386	1.00 31.45	В
,	ATOM	1333	C	LEU	182	25.581	22.690	68.260	1.00 33.98	В
					182	26.197				
	MOTA	1334	0	LEU			22.057	69.117	1.00 33.33	В
	MOTA	1335	N	GLN	183	24.259	22.843	68.266	1.00 33.26	В
10	MOTA	1336	CA	GLN	183	23.399	22.259	69.296	1.00 32.84	В
10	MOTA	1337	CB	GLN	183	22.430	23.320	69.842	1.00 34.22	В
	ATOM	1338	CG	GLN	183	23.122	24.542	70.436	1.00 37.39	В
	MOTA	1339	CD	GLN	183	22.163	25.699	70.671	1.00 38.77	В
	ATOM	1340		GLN	183	21.325	26.003	69.818	1.00 39.62	В
1.5	MOTA	1341		GLN	183	22.294	26.361	71.820	1.00 37.72	Ð
15	MOTA	1342	С	GLN	183	22.603	21.099	68.706	1.00 31.57	8
	MOTA	1343	0	GLN	183	22.209	21.134	67.545	1.00 31.18	В
	MOTA	1344	N	MET	184	22.353	20.079	69.513	1.00 31.59	В
	MOTA	1345	CA	MET	184	21.622	18.908	69.052	1.00 32.44	В
	ATOM	1346	CB	MET	184	22.480	17.677	69.297	1.00 32.63	В
20	ATOM	1347	CG	MET	184	22.018	16.404	68.626	1.00 34.09	В
	ATOM	1348	SD	MET	184	23.162	15.016	68.908	1.00 32.00	В
	MOTA	1349	CE	MET	184	22.574	14.436	70.488	1.00 31.68	В.
	ATOM	1350	С	MET	184	20.289	18.787	69.791	1.00 34.68	В
	MOTA	1351	0	MET	184	20.203	19.114	70.976	1.00 35.18	·B
25	MOTA	1352	N	PHE	185	19.248	18.345	69.086	1.00 36.66	В
	MOTA	1353	CA	PHE	185	17.922	18.168	69.690	1.00 39.01	В
	MOTA	1354	СВ	PHE	185	16.987	19.422	69.462	1.00 37.84	В
	MOTA	1355	CG	PHE	185	17:676	20.750	69.619	1.00 38.18	В
	ATOM	1356	CD1	PHE	185	18.453	21.270	68.593	1.00 36.50	В
30	ATOM	1357		PHE	185	17.534	21.488	70.793	1.00 38.31	В
	ATOM	1358		PHE	185	19.080	22.502	68.724	1.00 36.83	В
	MOTA	1359		PHE	185	18.158	22.724	70.936	1.00 38.32	В
	ATOM	1360	CZ	PHE	185	18.933	23.232	69.897	1.00 38.06	В
	ATOM	1361	C	PHE	185	17.224	16:956	69.077	1.00 40.70	В
35	ATOM	1362	ō	PHE	185	17.485	16.598	67.931	1.00 39.58	В
	ATOM	1363	N	ASP	186	16.333	16.330	69.838	1.00 43.77	В
	ATOM	1364	CA	ASP	186	15.588	15.187	69.328	1.00 46.67	B
	ATOM	1365	CB	ASP	186	14.737	14.550	70.419	1.00 47.89	В
	ATOM	1366	CG	ASP	186	15.534	14.206	71.659	1.00 50.45	В
40	ATOM	1367		ASP	186	16.535	13.461	71.540	1.00 50.63	В
. •	ATOM	1368		ASP	186	15.154	14.679	72.756	1.00 51.23	В
	ATOM	1369	C	ASP	186	14.668	15.740	68.262	1.00 47.79	B
	ATOM	1370	ō	ASP	186	14.371	16.933	68.246	1.00 47.04	В
	ATOM	1371	N	ASP	187	14.215	14.883	67.365	1.00 50.77	В
45	ATOM	1372	CA	ASP	187	13.318	15.351	66.328	1.00 54.90	В
	ATOM	1373	CB	ASP	187	13.748	14.832	64.990	1.00 56.93	В
	ATOM	1374	CG	ASP	187	12.973	15.457	63.860	1.00 59.28	В
	ATOM	1375		ASP	187	13.425	15.343	62.700	1.00 50.01	В
	MOTA	1376		ASP	187	11.910	16.060	64.138	1.00 60.38	В
50	MOTA	1377	C	ASP	187	11.915	14.877	66.662	1.00 56.34	В
50	MOTA	1378	Ö	ASP	187	11.638	13.678	66.649	1.00 56.08	В
	ATOM	1379	N	PRO	188	11.015			1.00 58.00	В
	MOTA		CD	PRO			15.820	66.985		
	ATOM	1380 1381	CA	PRO	188	11.251	17.274 15.529	66.963 67.339	1.00 57.99	В
55					188	9.621	16.890		1.00 60.11	В
55	MOTA	1382	CB	PRO	188	8.978		67.309	1.00 59.76	В
	MOTA	1383	CG	PRO	188	10.091	17.790	67.764	1.00 58.23	В
	MOTA	1384	C	PRO	188	8.956	14.549	66.376	1.00 61.87	B
	MOTA	1385	0	PRO	188	8.162	13.700	66.783	1.00 61.46	В
60	MOTA	1386	N	ARG	189	9.302	14.669	65.100	1.00 64.31	В
UU	ATOM	1387	CA	ARG	189	8:757	13.812	64.058	1.00 66.68	В
	MOTA	1388	CB	ARG	189	9.307	14.265	62.701	1.00 65.61	В
	MOTA	1389	CG	ARG	189	8.813	15.651	62.277	1.00 66.58	В
	MOTA	1390	CD	ARG	189	9.586	16.213	.61.080	1.00 66.65	В
c =	MOTA	1391	NĒ	ARG	189	10.834	16.866	61.474	1.00 66.32	В
65	MOTA	1392	CZ	ARG	189	11.704	17.407	60.625	1.00 66.09	В
	MOTA	1393	NH1		189	11.474	17.377	59.319	1.00 66.33	В
	MOTA	1394	NH2	ARG	189	12.803	17.988	61.083	1.00 65.55	В
	MOTA	1395	С	ARG	189	9.041	12.321	64.289	1.00 68.64	В
	MOTA	1396	0	ARG	189	8.300	11.461	63.813	1.00 69.00	В
70	MOTA	1397	N	ASN	190	10.110	12.018	65.022	1.00 71.07	В
	ATOM	1398	CA	ASN	190	10.487	10.634	65.329	1.00 72.28	В
	ATOM	1399	CB	ASN	190	10.758	9.814	63.998	1.00 72.30	В
	MOTA	1400	CG	ASN	190	11.706	10.525	63.041	1.00 71.90	В
	-	-			-			· 		_

	MOTA	1401	OD1	ASN	190	12.847	10.822	63.385	1.00 71.47	В
	MOTA	1402	ND2	ASN	190	11.233	10.789	61.826	1.00 71.27	В
	MOTA	1403	С	ASN	190	11.709	10.579	66.252	1.00 73.09	В
	MOTA	1404	ō	ASN	190	12.783	11.067	65.905	1.00 73.71	В
5	ATOM	1405	N	LYS	191	11.534	9.979	67.427	1.00 73.58	В
,								68.428	1.00 73.23	В
	MOTA	1406	CA	LYS	191	12.601	9.871			
	MOTA	1407	CB	LYS	191	12.123	9.021	69.606	1.00 75.05	В
	MOTA	1408	CG	LYS	191	11.285	9.778	70.614	1.00 76.84	В
	MOTA	1409	CD	LYS	191	12.074	10.920	71.241	1.00 77.87	В
10	ATOM	1410	CΕ	LYS	191	11.299	11.547	72.387	1.00 78.94	В
	ATOM	1411	NZ	LYS	191	9.939	11.988	71.961	1.00 79.06	В
	MOTA	1412	c	LYS	191	13.965	9.351	67.968	1.00 71.65	В
	MOTA	1413	ō	LYS	191	15.000	9.869	68.395	1.00 71.97	В
1.5	MOTA	1414	N	ARG	192	13.977	8.326	67.121	1.00 68.70	В
15	MOTA	1415	CA	arg	192	15.238	7.772	66.638	1.00 65.72	В
	MOTA	1416	CB	arg	192	14.978	6.515	65.768	1.00 67.67	В
	MOTA	1417	CG	ARG	192	16.217	5.978	65.052	1.00 69.51	В
	MOTA	1418	CD	ARG	192	16.068	4.519	64.616	1.00 70.83	В
	MOTA	1419	NE	ARG	192	14.855	4.261	63.839	1.00 71.87	В
20	ATOM	1420	CZ	ARG	192	13.672	3.950	64.364	1.00 71.73	В
20		1421	NH1		192	13.527	3.855	65.681	1.00 70.61	В
	MOTA									
	MOTA	1422	NH2		192	12.631	3.727	63.569	1.00 71.53	В
	MOTA	1423	С	ARG	192	16.033	8.803	65.843	1.00 62.08	В
~-	ATOM	1424	0	ARG	192	17.190	8.572	65.482	1.00 61.32	₿
25	MOTA	1425	N	GLY	193 -	15.403	9.946	65.585	1.00 58.42	В
	MOTA	1426	CA	GLY	193	16.045	11.008	64.828	1.00 52.07	В
	ATOM	1427	С	GLY	193	16.519	12.171	65.674	1.00 47.14	В
	MOTA	1428	ō	GLY	193	16.159	12.300	66.843	1.00 46.94	В
	ATOM	1429	N	VAL	194	17.323	13.033	65.067	1.00 44.16	В
30										В
20	MOTA	1430	CA	VAL	194	17.875	14.184	65.757	1.00 40.67	
	MOTA	1431	CB	VAL	194	19.266	13.838	66.329	1.00 39.96	В
	MOTA	1432	CG1	VAL	194	20.338	14.058	65.271	1.00 37.96	В
	MOTA	1433	CG2	VAL	194 .	19.539	14.653	67.564	1.00 39.63	В
	MOTA	1434	С	VAL	194	18.008	15.373	64.800	1.00 39.90	В
35	MOTA	1435	0	VAL	194	18.145	15.194	63.592	1.00 40.91	В
	MOTA	1436	N	ILE	195	17.965	16.585	65.347	1.00 38.55	В
	ATOM	1437	CA	ILE	195	18.104	17.803	64.553	1.00 35.81	В
							18.728		1.00 38.25	В
	MOTA	1438	CB	ILE	195	16.862		64.709		
40	MOTA	1439	CG2		195	17.132	20.092	64.055	1.00 38.19	В
40	MOTA	1440	CG1		195	15.615	18.049	64.084	1.00 39.77	В
•	ATOM	1441	CD1	ILE	195	14.321	18.863	64.185	1.00 41.59	В
	MOTA	1442	С	ILE	195	19.347	18.581	65.001	1.00 32.57	В
	MOTA	1443	0	ILE	195	19.452	18.970	66.162	1.00 30.74	В
	MOTA	1444	N	ILE	196	20.292	18.787	64.086	1.00 29.82	В
45	ATOM	1445	CA	ILE	196	21.500	19.539	64.405	1.00 27.94	В
73								63.769		В
	MOTA	1446	CB	ILE	196	22.800	18.919		1.00 26.64	
	MOTA	1447	CG2		196	24.006	19.816	64.070	1.00 21.22	В
	MOTA	1448	CG1		196	23.110	17.510	64.383	1.00 24.18	В
	MOTA	1449	CD1	ILE	196	22.375	16.374	63.764	1.00 22.10	В
50	ATOM	1450	С	ILE	196	21.303	20.951	63.872	1.00 27.99	В
	MOTA	1451	0	ILE	196	21.375	21.196	62.669	1.00 27.68	В
	MOTA	1452	N	LYS	197	21.044	21.876	64.784	1.00 29.44	В
	ATOM	1453	CA	LYS	197	20.813	23.265	64.426	1.00 30.91	В
	ATOM	1454	CB	LYS	197	20.205	24.026	65.616	1.00 33.42	В
55	ATOM								1.00 35.76	В
55		1455	CG	LYS	197	19.931	25.486	65.303		
	MOTA	1456	CD	LYS	197	19.670	26.299	66.548	1.00 39.21	В
	MOTA	1457	CE	LYS	197	19.686	27.776	66.199	1.00 42.14	В
	ATOM	1458	NZ	LYS	197	20.909	28.121	65.411	1.00 42.07	В
	MOTA	1459	С	LYS	197	22.073	23.984	63.971	1.00 29.67	В
60	MOTA	1460	0	LYS	197	23.080	23.977	64.674	1.00 29.22	В
••	MOTA	1461	N		198	22.005	24.600	62.792	1.00 29.85	В
				GLY						
	MOTA	1462	CA	GLY	198	23.141	25.345	62.275	1.00 30.66	В
	MOTA	1463	С	GLY	198	24.040	24.637	61.282	1.00 30.74	В
15	MOTA	1464	0	GLY	198	24.857	25.283	60.618	1.00 30.16	В
65	MOTA	1465	N	LEU	199	23.903	23.318	61.178	1.00 30.32	В
	MOTA	1466	CA	LEU	199	24.722	22.538	60.255	1.00 30.74	В
	ATOM	1467	CB	LEU	199	24.530	21.004	60.530	1.00 30.24	В
	ATOM	1468	CG	LEU	199	25.328	19.967	59.664	1.00 28.88	. B
									1.00 30.22	
70	ATOM	1469	CD1		199	26.773	20.398	59.527		В
70	ATOM	1470			199	25.254	18.587	60.308	1.00 28.26	В
	MOTA	1471	C	LEU	199	24.397	22.869	58.792	1.00 31.25	В
	ATOM	1472	0	LEU	199	23.256	22.699	58.340	1.00 31.36	В
	MOTA	1473	N	GLU	200	25.406	23.345	58.065	1.00 30.26	В

	MOTA	1474	CA	GLU	200	25.253	23.712	56.661	1.00 32.06	В
	MOTA	1475	CB	GLU	200	26.446	24.590	56.190	1.00 34.38	В
	ATOM	1476	CG	GLU	200	26.604	25.870	56.961	1.00 41.33	В
	ATOM	1477	CD	GLU	200	25.395	26.773	56.833	1.00 42.76	В
5	ATOM	1478	OE1		200	25.121	27.535	57.785	1.00 43.19	В
-	MOTA	1479	OE2		200	24.730	26.721	55.776	1.00 43.56	В
	MOTA	1480	C	GLU	200	25.164	22.514	55.722	1.00 31.83	В
	MOTA	1481	õ	GLU	200	25.841	21.503	55.916	1.00 30.83	В
	MOTA	1482	N	GLU	201	24.328	22.654	54.700	1.00 30.84	В
10			CA	GLU	201		21.639	53.677	1.00 30.37	В
10	MOTA	1483		GLU		24.163		-		. В
	MOTA	1484	CB		· 201 201	22.732	21.167	53.611	1.00 30.91	В
	ATOM	1485	CG	GLU		22.386	20.111	54.629		В
	MOTA	1486	CD	GLU	201	20.975	19.587	54.454	1.00 36.02	В
15	MOTA MOTA	1487		GLU	201 201	20.052 20.791	20.163	55.069	1.00 37.16	B
13		1488		GLU			18.604	53.695	1.00 30.36	В
	MOTA	1489	C	GLU	201	24.528	22.328	52.373	1.00 30.44	В
	MOTA	1490 1491	0	GLU	201	23.796	23.207 21.958	51.919		В
	MOTA	1491	N	ILE	202	25.663 26.073		51.783	1.00 28.80	B
20	MOTA		CA	ILE	202		22.575	50.526 50.409	1.00 28.82 1.00 28.91	В
20	ATOM	1493	CB		202	27.619	22.739			В
	MOTA	1494		ILE	202	27.978	23.225	49.014	1.00 26.00 1.00 28.90	В.
	MOTA	1495		ILE	202	28.137	23.751	51.426		В.
	MOTA	1496		ILE	202	28.057	23.294	52.863	1.00 32.03	В
25	MOTA	1497	C	ILE	202	25.594	21.773	49.324	1.00 28.57	
25	MOTA	1498	0	ILE	202	25.844	20.571	49.215	1.00 29.93	B B
	MOTA	1499 1500	N	THR	203	24.896	22.448	48.422	1.00 28.23	В
	MOTA		CA	THR	203	24.404	21.803	47.219	1.00 26.49	В
	ATOM	1501	CB	THR	203	23.307	22.665	46.527	1.00 26.14	
30	MOTA	1502		THR	203	22.173	22.791	47.401	1.00 24.25	В
λO	MOTA	1503		THR	203	22.862	22.028	45.208	1.00 25.01	В
	MOTA	1504	C	THR	203	25.606	21.636	46.293	1.00 26.13	В
	MOTA	1505	0	THR	203	26.483	22.495	46.253	1.00 26.91	В
	ATOM	1506	N	VAL	204	25.666	20.504	45.599	1.00 26.49	В
35	ATOM	1507	CA	VAL	204	26.741	20.220	44.654	1.00 27.51	В
22	MOTA	1508	CB	VAL	204	27.444	18.868	44.967	1.00 25.76	В
	ATOM	1509		VAL	204	28.653	18.672	44.056	1.00 23.12	В
	MOTA	1510		VAL	204	27.879	18.837	46.423	1.00 24.79	В
	MOTA	1511	C	VAL	204		. 20.149	43.321	1.00 29.14	В
40	MOTA	1512	0	VAL	204	25.265	19.199	43.061		B B
40	MOTA	1513	N	HIS	205	26.218	21.170	42.495	1.00 29.22	B
	MOTA	1514	CA	HIS	205	25.553	21.313	41.195		
	MOTA	1515	CB	HIS	205	25.613	22.794	40.767	1.00 28.34	B B
	MOTA	1516	CG	HIS	205	25.157	23.732	41.838	1.00 28.46	В
45	ATOM	1517 1518		HIS	205	25.858	24.492	42.711 42.196	1.00 27.43	В
73	MOTA MOTA	1519		HIS	205 205	23.832	23.862	43.249	1.00 28.44	В
	MOTA	1520		HIS	205	23.736 24.952	24.654 25.049	43.582	1.00 29.92	В
	MOTA	1521	C	HIS	205	26.092	20.435	40.081	1.00 31.51	В
	MOTA	1522	0	HIS	205	25.358	20.055	39.169	1.00 31.34	В
50	MOTA	1523	N	ASN	206	27.383	20.136	40.147	1.00 33.49	В
. 30	MOTA	1524	CA	ASN	206	28.032	19.299	39.151	1.00 34.62	В
	MOTA	1525	CB	ASN	206	28.444	20.138	37.930	1.00 34.75	В
	MOTA	1526	CG	ASN	206	29.164	21.417	38.309	1.00 35.27	B
	ATOM	1527	OD1	ASN	206	30.224	21.391	38.938	1.00 37.58	В
55	MOTA	1528		ASN	206	28.589	22.548	37.925	1.00 34.11	B
-	MOTA	1529	C	ASN	206	29.243	18.650	39.798	1.00 35.69	В
	ATOM	1530	ò	ASN	206	29.478	18.836	40.992	1.00 36.45	B
	MOTA	1531	N	LYS	207	30.002	17.876	39.031	1.00 36.43	В.
	MOTA	1532	CA	LYS	207	31.171	17.216	39.590	1.00 38.62	В
60	ATOM	1533	СВ	LYS	207	31:582	15.993	38.703	1.00 40.10	В
00	MOTA	1534	CG	LYS	207		16.339	37.319	1.00 42.56	8
	ATOM	1535	CD	LYS	207	32.259	15.081	36.456	1.00 44.26	8
	ATOM									
	ATOM	1536 1537	CE NZ	LYS	207 207	33.191 34.613	15.293 15.454	35.267 35.696	1.00 43.78	B B
65	ATOM	1538		LYS		32.313	18.222	39.700	1.00 42.48	В
55			С 0	LYS	207	33.176	18.120	40.576	1.00 39.03	В
	ATOM ATOM	1539 1540		LYS	207			38.813	1.00 38.73	В
	ATOM	1540	N	ASP	208	32.292 33.312	19.208	38.790	1.00 40.76	В
		1542	CA		208 208	33.312	20.244	37.461	1.00 40.78	В
70	MOTA		CB	ASP	208		20.981 20.101	36.292	1.00 42.38	В
	MOTA MOTA	1543		ASP	208	33.659	20.101	35.127	1.00 45.31	В
	MOTA	1544		ASP	208	33.407 34.246	19.023	36.542	1.00 46.78	В
	ATOM	1545	C		208 208		21.219	39.952	1.00 46.78	В
	MION	1546	·	ASP	208	33.141	41.413	33.336	1.00 33.33	

	MOTA	1547	0	ASP	208	33.643	22.339	39.922	1.00 41.22	В
	MOTA	1548	N	GLU	209	32.457	20.784	40.996	1.00 37.46	В
	ATOM	1549	CA	GLU	209	32.241	21.660	42.128	1.00 35.89	В
	ATOM	1550	СВ	GLU	209	30.760	22.075	42.158	1.00 35.84	В
5	MOTA	1551	CG	GLU	209	30.445	23.275	43.010	1.00 37.17	В
•	ATOM	1552	CD	GLU	209	28.973	23.682	42.924	1.00 38.94	В
	ATOM	1553		GLU	209			41.793	1.00 37.72	В
						28.462	23.857			
	ATOM	1554	OE2		209	28.327	23.835	43.988	1.00 38.77	В
10	MOTA	1555	Ç	GLU	209	32.646	20.992	43.439	1.00 34.61	В
10	MOTA	1556	0	GLU	209	32.763	21.657	44.470	1.00 36.51	В
	MOTA	1557	N	VAL	210	32.907	19.690	43.395	1.00 32.07	В
	ATOM	1558	CA	VAL	210	33.268	18.966	44.609	1.00 29.92	В
	ATOM	1559	CB	VAL	210	33.065	17.411	44.450	1.00 29.01	В
	MOTA	1560	CG1	VAL	210	31.856	17.110	43.574	1.00 26.09	В
15	ATOM	1561	CG2		210	34.301	16.774	43.901	1.00 29.03	В
	ATOM	1562	c	VAL	210	34.668	19.212	45.183	1.00 28.45	В
	ATOM	1563	ō	VAL	210	34.820	19.322	46.406	1.00 29.31	В
	ATOM	1564	N	TYR	211	35.694	19.311	44.343	1.00 26.40	В
20	MOTA	1565	CA	TYR	211	37.038	19.505	44.894	1.00 24.93	В
20	MOTA	1566	CB	TYR	211	38.106	19.552	43.783	1.00 22.02	В
	ATOM	1567	CG	TYR	211	39.510	19.386	44.318	1.00 23.83	В
	MOTA	1568		TYR	211	39.850	18.284	45.097	1.00 26.06	В
	ATOM	1569	CE1		211	41.136	18.131	45.625	1.00 25.76	В
~-	MOTA	1570	CD2	TYR	211	40.498	20.339	44.074	1.00 24.90	В
25	MOTA	1571	CE2	TYR	211	41.790	20.196	44.597	1.00 24.81	В
	MOTA	1572	CZ	TYR	211	42.103	19.089	45.374	1.00 25.75	В
	ATOM	1573	ОН	·TYR	211	43.373	18.938	45.910	1.00 23.97	В
	ATOM	1574	С	TYR	211	37.111	20.759	45.757	1.00 25.45	В
	ATOM	1575	Ō	TYR	211	37.691	20.740	46.844	1.00 24.21	В
30	ATOM	1576	N	GLN	212	36.501	21.840	45.272	1.00 27.99	В
-	MOTA	1577	CA	GLN	212	36.473	23.117	45.983	1.00 27.45	В
	ATOM	1578	CB	GLN	212	35.721	24.126		1.00 31.66	В
				GLN				45.163		
	ATOM	1579	CG		212	35.365	25.402	45.907	1.00 37.63	В
35	ATOM	1580	CD	GLN	212	35.696	26.654	45.105	1.00 40.53	В
22	ATOM	1581		GLN	212	35.305	26.782	43.937	1.00 39.59	В
	MOTA	1582	NE2		212	36.418	27.587	45.731	1.00 39.73	В
	ATOM	1583	С	GLN	212	35.834	22.981	47.364	1.00 26.73	В
	MOTA	1584	0	GLN	212	36.329	23.527	48.347	1.00 26.01	В
40	MOTA	1585	N	ILE	213	34.733	22.243	47.437	1.00 26.10	B
40	MOTA	1586	CA	ILE	213	34.044	22.037	48.703	1.00 24.91	В
	MOTA	1587	CB	ILE	213	32.694	21.327	48.496	1.00 23.51	В
	ATOM	1588	CG2	ILE	213	31.978	21.200	49.835	1:00 20.39	В
	ATOM	1589		ILE	213	31.843	22.117	47.461	1.00 22.89	В
	MOTA	1590		ILE	213	30.472	21.509	47.152	1.00 23.13	В
45	ATOM	1591	c	ILE	213	34.906	21.207	49.656	1.00 25.49	В
	MOTA	1592	ō	ILE	213	34.916	21.448	50.865	1.00 24.30	В
	ATOM	1593	N	LEU	214	35.618	20.226	49.106	1.00 26.92	В
	ATOM	1594	CA	LEU	214	36.496	19.381	49.905	1.00 28.08	В
	ATOM	1595	CB	LEU	214		18.168		1.00 28.00	В
50						37.031		49.050		
50	MOTA	1596	CG	LEU	214	36.272	16.802	49.152	1.00 30.13	В
	MOTA	1597		LEU	214	34.796	17.034	49.411	1.00 31.20	В
	ATOM	1598		LEU	214	36.482	15.987	47.876	1.00 29.12	В
	MOTA	1599	C	LEU	214	37.657	20.225	50.442	1.00 29.28	В
E E	MOTA	1600	0	LEU	214	38.012	20.114	51.620	1.00 30.45	В
55	MOTA	1601	N	GLU	215	38.235	21.083	49.599	1.00 28.08	В
	MOTA	1602	CA	GLU	215	39.339	21.932	50.059	1.00 28.89	В
	MOTA	1603	CB	GLU	215	39.864	22.842	48.914	1.00 29.69	В
	MOTA	1604	CG	GLU	215	40.426	22.093	47.714	1.00 33.51	В
	ATOM.	1605	CD	GLU	215	41.092	23.014	46.700	1.00 36.27	В
60	MOTA	1606	0E1	GLU	215	42.343	23.136	46.730	1.00 34.34	В
	MOTA	1607		GLU	215	40.358	23.620	45.880	1.00 36.57	В
	ATOM	1608	c	GLU	215	38.919	22.795	51.255	1.00 28.03	В
	ATOM	1609	ŏ	GLU	215	39.682	22.953	52.210	1.00 27.31	В
	ATOM	1610	N	LYS	216	37.707	23.348	51.204	1.00 27.31	
65				LYS						.B
U)	MOTA	1611	CA		216	37.202	24.183	52.290	1.00 29.52	В
	MOTA	1612	CB	LYS	216	35.799	24.696	51.971	1.00 30.11	В
	MOTA	1613	CG	LYS	216	35.691	25.416	50.650	1.00 32.53	В
	MOTA	1614	CD	LYS	216	36.584	26.643	50.602	1.00 34.31	В
70	MOTA	1615	CE	LYS	216	36.596	27.272	49.200	1.00 36.64	, B
70	MOTA	1616	NZ	LYS	216	37.248	26.419	48.152	1.00 34.44	В
	ATOM	1617	С	LYS	216	37.170	23.415	53.609	1.00 30.05	В
	ATOM	1618	0	LYS	216	37.516	23.960	54.658	1.00 31.96	В
	MOTA	1619	N	GLY	217	36.742	22.156	53.553	1.00 30.83	В

	MOTA	1620	CA	GLY	217	36.695	21.335	54.752	1.00 29.82	В
	MOTA	1621	С	GLY	217	38.107	21.144	55.270	1.00 29.77	В
	ATOM	1622	Ō	GLY	217	38.389	21.354	56.460	1.00 28.73	В
-	MOTA	1623	N	ALA	218	39.000	20.749	54.363	1.00 29.20	В
5	MOTA	1624	CA	ALA	218	40.404	20.548	54.696	1.00 28.09	. В
	MOTA	1625	CB	ALA	218	41.212	20.299	53.427	1.00 25.39	В
									1.00 27.61	В
	MOTA	1626	С	ALA	218	40.924	21.792	55.422		
	ATOM	1627	0	ALA	218	41.623	21.684	56.429	1.00 27.17	₿
	MOTA	1628	N	ALA	219	40.559	22.969	54.914	1.00 27.54	В
10							24.243	55.505	1.00 27.45	В
10	MOTA	1629	CA	ALA	219	40.984				
	MOTA	1630	CB	ALA	219	40.430	25.406	54.695	1.00 26.20	В
	MOTA	1631	С	ALA	219	40.553	24.385	56.964	1.00 27.16	В
	MOTA	1632	0	ALA	219	41.368	24.726	57.833	1.00 26.05	В
15	MOTA	1633	N	LYS	220	39.273	24.135	57.227	1.00 26.17	В
15	MOTA	1634	CA	LYS	220	38.754	24.234	58.585	1.00 26.59	В
	MOTA	1635	CB	LYS	220	37.203	24.057	58.592	1.00 25.82	В
	ATOM	1636	CG	LYS	220	36.477	25.037	57.691	1.00 26.36	В
	MOTA	1637	CD	LYS	220	34.997	25.195	58.065	1.00 28.61	В
	MOTA	1638	CΕ	LYS	220	34.827	25.771	59.471	1.00 27.13	В
20	ATOM	1639	NZ	LYS	220	33.406	26.129	59.789	1.00 25.98	В
	MOTA	1640	c	LYS	220	39.426	23.190	59.491	1.00 26.00	В
	ATOM	1641	0	LYS	220	39.715	23.465	60.665	1.00 24.88	В.
	ATOM	1642	N	ARG	221	39.671	22.000	58.937	1.00 24.80	В
	ATOM	1643	CA	ARG	221	40.330	20.916	59.671	1.00 22.73	В
25										В
23	MOTA	1644	CB	ARG	221	40.685	19.757	58.725	1.00 24.70	
	MOTA	1645	CG	ARG	221	39.524	18.885	58.293	1.00 25.62	В
	MOTA	1646	CD	ARG	221	39.367	17.736	59.256	1.00 26.10	В
	ATOM	1647	NE	ARG	221	38:190	16.934	58.960	1.00 24.76	В
20	ATOM	1648	CZ	ARG	221	38.065	16.146	57.901	1.00 22.87	В
30	ATOM	1649	NH1	ARG	221	39.061	16.051	57.021	1.00 19.50	В
	MOTA	1650	NH2	ARG	221	36.942	15.451	57.735	1.00 20.09	В
	ATOM	1651	C	ARG	221	41.624	21.456	60.267	1.00 21.95	В
	MOTA	1652	0	ARG	221	41.889	21.306	61.456	1.00 20.88	В
	ATOM	1653	N	THR	222	42.421	22.089	59.406	1.00 20.21	В
35	MOTA	.1654	CA	THR	222	43.705	22.661	59.795	1.00 19.39	В
	ATOM	1655	CB	THR	222	44.312	23.464	58.650	1.00 21.09	В
	MOTA	1656	OG1	THR	222	44.502	22.600	57.525	1.00 22.38	В
	ATOM	1657	CG2	THR	222	45.649	24.077	59.073	1.00 20.44	В
	MOTA	1658	C	THR	222	43.589	23.579	60.991	1.00 18.28	В
40		1659						61.952	1.00 17.80	В
70	MOTA		0	THR	222	44.338	23.441			
	MOTA	1660	N	THR	223	42.649	24.517	60.926	1.00 17.37	В
	ATOM	1661	CA	THR	223	42.452	25.461	62.012	1.00 18.66	В
	MOTA	1662	CB	THR	223	41.496	26.590	61.605	1.00 17.71	В
	ATOM	1663	OG1	THR	223	40.245	26.413	62.268	1.00 20.08	В
45										
43	MOTA	1664	CG2		223	41.258	26.581	60.111	1.00 16.54	В
	ATOM	1665	С	THR	223	41.902	24.740	63.242	1.00 20.76	В
	MOTA	1666	0	THR	223	42.206	25.120	64.374	1.00 24.08	В
	ATOM	1667	N	ALA	224	41.100	23.698	63.018	1.00 21.47	В
- 0	MOTA	1668	CA	ALA	224	40.529	22.898	64.105	1.00 19.87	В
50	ATOM	1669	CB	ALA	224	39.642	21.801	63.534	1.00 22.14	В
	MOTA	1670	С	ALA	224	41.667	22.266	64.894	1.00 19.87	В
	MOTA	1671	ō	ALA	224	41.689	22.289	66.129	1.00 16.71	В
	ATOM	1672	N	ALA	225	42.604	21.680	64.155	1.00 20.37	В
	MOTA	1673	CA	ALA	225	43.765	21.048	64.755	1.00 20.88	В
55	MOTA	1674	CB	ALA	225	44.647	20.440	63.666	1.00 19.50	В
-				ALA		44.541	22.096	65.553	1.00 22.18	В
	MOTA	1675	С		225					
	MOTA	1676	0	ALA	225	45.054	21.808	66.638	1.00 20.94	B
	ATOM	1677	N	THR	226	44.613	23.319	65.023	1.00 23.92	₿.
	MOTA	1678	CA	THR	226	45.324	24.401	65.717	1.00 24.83	В
60	MOTA									В
50		1679	CB	THR	226	45.313	25.723	64.895	1.00 24.59	
	MOTA	1680	OG1	THR	226	46.088		63.699	1.00 23.18	В
	MOTA	1681	CG2	THR	226	45.904	26.866	65.721	1.00 25.23	B
	MOTA	1682	C	THR	226	44.699	24.679	67.089	1.00 25.41	В
		1683				45.405		68.083		
65	MOTA		0	THR	226		24.877		1.00 25.12	В
65	MOTA	1684	N	LEU	227	43.370	24.680	67.130	1.00 25.47	В
	MOTA	1685	CA	LEU	227	42.619	24.942	68.353	1.00 26.90	В
	ATOM	1686	CB	LEU	227	41.222	25.541	67.980	1.00 29.00	В
		1687							1.00 32.68	
	MOTA		CG	LEU	227	41.051	27.041	67.561		В
70	ATOM	1688	CD1	LEU	227	42.240	27.567	66.763	1.00 31.51	В
70	ATOM	1689	CD2	LEU	227	39.756	27.156	66.755	1.00 32.75	В
	ATOM	1690	c	LEU	227	42.409	23.739	69.296	1.00 26.44	В
	ATOM	1691	0	LEU	227	42.348	23.906	70.520	1.00 25.50	В
	MOTA	1692	N	MET	228	42.295	22.533	68.755	1.00 24.99	В

	MOTA	1693	CA	MET	228	42.041	21.392	69.635	1.00 25.58	В
	MOTA	1694	CB	MET	228	40.625	20.786	69.310	1.00 27.00	В
							21.798	69.554	1.00 28.30	В
	ATOM	1695	CC	MET	228	39.499				
_	MOTA	1696	SD	MET	228	37.874	21.368	68.919	1.00 31.74	В
5	MOTA	1697	CE	MET	228	37.998	22.026	67.265	1.00 30.21	В
-	MOTA	1698	c	MET	228	43.091	20.301	69.666	1.00 23.55	В
									1.00 23.83	В
	MOTA	1699	0	MET	228	43.547	19.828	68.629		
	MOTA	1700	N	ASN	229	43.471	19.913	70.882	1.00 22.85	В
	MOTA	1701	CA	ASN	229	44.470	18.870	71.099	1.00 21.02	В
10	ATOM	1702	СВ	ASN	229	44.574	18.524	72.588	1.00 19.32	В
10										В
	MOTA	1703	CG	ASN	229	45.172	19.646	73.426	1.00 19.33	
	MOTA	1704	OD1	ASN	229	45.690	20.634	72.899	1.00 19.44	В
	MOTA	1705	ND2	ASN	229	45.112	19.484	74.751	1.00 13.92	В
	ATOM	1706	С	ASN	229	44.162	17.582	70.329	1.00 21.09	В
15					229	43.063	17.026	70.435	1.00 21.09	В
13	MOTA	1707	0	ASN						
	MOTA	1708	N	ALA	230	45.144	17.121	69.55B	1.00 20.25	В
	ATOM	1709	CA	ALA	230	45.030	15.887	68.786	1.00 19.42	В
	MOTA	1710	CB	ALA	230	45.224	14.675	69.721	1.00 21.67	В
	MOTA	1711	ç	ALA	230	43.694	15.783	68.067	1.00 18.26	В
20										B
20	MOTA	1712	0	ALA	230	43.096	14.712	68.000	1.00 17.83	
	MOTA	1713	N	TYR	231	43.242	16.897	67.512	1.00 17.17	В
	MOTA	1714	CA	TYR	231	41.965	16.927	66.821	1.00 17.72	В
	MOTA	1715	СВ	TYR	231	41.694	18.379	66.201	1.00 15.95	В
										В
25	MOTA	1716	cc	TYR	231	40.341	18.465	65.524	1.00 12.55	
25	ATOM	1717	CD1	TYR	231	40.205	18.269	64.151	1.00 12.28	• В
	MOTA	1718	CE1	TYR	231	38.933	18.219	63.555	1.00 8.18	В
	ATOM	1719		TYR	231	39.182	18.621	66.279	1.00 10.61	В
								65.690	1.00 9.26	В
	MOTA	1720		TYR	231	37.918	18.573			
	MOTA	1721	CZ	TYR	231	37.802	18.372	64.338	1.00 6.19	В
30	MOTA	1722	ОН	TYR	231	36.545	18.335	63.777	1.00 8.98	В
	MOTA	1723	C	TYR	231	41.728	15.869	65.731	1.00 18.14	В
							15.392	65.571	1.00 17.92	В
	MOTA	1724	0	TYR	231	40.596				
	MOTA	1725	N	SER	232	42.769	15.504	64.982	1.00 17.34	В
	MOTA	1726	CA	SER	232	42.585	14.537	63.903	1.00 17.96	В
35	MOTA	1727	CB	SER	232	43.681	14.688	62.B16	1.00 13.72	В
			OG		232		14.251	63.275	1.00 15.73	В
	MOTA	1728		SER		44.941				
	MOTA	1729	С	SER	232	42.502	13.070	64.323	1.00 18.78	В
	MOTA	1730	0	SER	232	41.934	12.255	63.598	1.00 19.24	В
	MOTA	1731	N	SER	233	43.051	12.726	65.480	1.00 17.77	В
40	ATOM	1732	CA	SER	233	43.019	11.340	65.904	1.00 16.56	В
70										B
	MOTA	1733	CB	SER	233	44.383	10.932	66.496	1.00 18.00	
	MOTA	1734	OG	SER	233	44.509	11.362	67.846	1.00 17.89	В
	MOTA	1735	С	SER	233	41.935	11.141	66.943	1.00 17.20	B
	MOTA	1736	ō	SER	233	41.413	10.035	67.110	1.00 13.55	В
45										В
40	MOTA	1737	N	ARG	234	41.570	12.235	67.609	1.00 18.37	
	MOTA	1738	CA	ARG	234	40.579	12.185	68.678	1.00 18.14	B
	ATOM	1739	CB	ARG	234	41.035	13.079	69.848	1.00 20.04	В
	ATOM	1740	CG	ARG	234	41.136	12.352	71.169	1.00 23.36	В
		1741	CD	ARG	234	42.547	12.392	71.767	1.00 25.39	В
50	MOTA									
<i>3</i> 0	MOTA	1742	NE	ARG	234	42.847	13.651	72.455	1.00 28.46	В
	MOTA	1743	CZ	ARG	234	43.898	13.844	73.255	1.00 28.83	В
	MOTA	1744	NH1		234	44.765	12.865	73.479	1.00 28.24	В
	ATOM	1745		ARG	234	44.082	15.019	73.842	1.00 28.56	В
								68.318	1.00 17.12	В
CE	MOTA	1746	C	ARG	234	39.142	12.524			
55	MOTA	1747	0	ARG	234	38.262	12.440	69.174	1.00 16.45	В
	MOTA	1748	N	SER	235	38.879	12.876	67.064	1.00 17.25	В
	ATOM	1749	CA	SER	235	37.508	13.232	66.685	1.00 17.01	В
										В
	MOTA	1750	CB	SER	235	37.470	14.581	66.108	1.00 16.15	
	ATOM	1751	OG	SER	235	38.109	14.594	64.847	1.00 15.24	В
60	ATOM	1752	С	SER	235	36.847	12.297	65.697	1.00 17.23	В
		1753	_			37.505	11.536	64.991	1.00 17.87	В
	MOTA		0	SER	235					
	MOTA	1754	N	HIS	236	35.527	12.381	65.655	1.00 16.90	В
	MOTA	1755	CA	HIS	236	34.720	11.580	64.750	1.00 18.47	В
	MOTA	1756	CB	HIS	236	33.553	10.961	65.484	1.00 20.05	В
65	ATOM	1757	CG	HIS	236	33.941	10.192	66.705	1.00 21.39	В
55										
	MOTA	1758		HIS	236	33.907	10.529	68.016	1.00 20.87	В
	MOTA	1759		HIS	236	34.444	8.910	66.650	1.00 21.00	В
	MOTA	1760	CE1	HIS	236	34.700	8.490	67.876	1.00 20.80	В
	MOTA	1761		HIS	236	34.385	9.454	68.723	1.00 19.15	В
70										
/U	MOTA	1762	С	HIS	236	34.166	12.518	63.688	1.00 19.93	В
	MOTA	1763	0	HIS	236	33.598	13.569	64.005	1.00 18.38	В
	MOTA	1764	N	SER	237	34.326	12.155	62.425	1.00 20.64	В
	MOTA	1765	CA	SER	237	33.795	13.001	61.374	1.00 21.44	В
	011	1,03	~"		~-,	22.123		02.3.4	2.00 21.47	-

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	MOTA	1766	CB	SER	237	34.889	13.424	60.424	1.00 20.		В
	MOTA	1767	OG	SER	237	35.258	12.370	59.566	1.00 19.	.17	В
	ATOM	176B	С	SER	237	32.731	12.224	60.619	1.00 21.	.91	В
	MOTA	1769	0	SER	237	32.908	11.043	60.320	1.00 21.	.18	В
5	ATOM	1770	N	VAL	238	31.620	12.886	60.324	1.00 21		В
•	ATOM	1771	CA	VAL	238	30.548	12.246	59.587	1.00 22		В
											В
	MOTA	1772	CB	VAL	238	29.297	12.024	60.475	1.00 25		
	MOTA	1773		VAL	238	29.043	13.241	61.323	1.00 27.		В
	MOTA	1774	CG2	VAL	238	28.077	11.717	59.601	1.00 24	.91	В
10	MOTA	1775	С	VAL	238	30.176	13.052	58.366	1.00 21.	. 64	В
	MOTA	1776	٠0	VAL	238	29.399	13.986	58.450	1.00 24.	.16	В
	ATOM	1777	N	PHE	239	30.764	12.683	57.232	1.00 23.		B
	ATOM	1778	CA	PHE	239	30.513	13.331	55.943	1.00 23		В
									1.00 22		
15	MOTA	1779	CB	PHE	239	31.736	13.139	55.002			В
15	MOTA	1780	ÇG	PHE	239	31.658	13.923	53.722	1.00 20		В
	MOTA	1781	CD1	PHE	239	30.660	13.667	52.785	1.00 19.		В
	MOTA	1782	CD2	PHE	239	32.580	14.92B	53.458	1.00 20.	- 63	В
	MOTA	1783	CE1	PHE	239	30.578	14.403	51.596	1.00 21	. 05	В
	MOTA	1784	CE2	PHE	239	32.510	15.676	52.268	1.00 21	.14	В
20	ATOM	1785	CZ	PHE	239	31.506	15.413	51.334	1.00 19		В
	ATOM	1786	č	PHE	239	29.286	12.669	55.321	1.00 24		B
						29.326		54.983			В.
	ATOM	1787	0	PHE	239		11.482		1.00 24		
	MOTA	1788	N	SER	240	28.202	13.430	55.178	1.00 24		8
25	MOTA	1789	CA	SER	240	26.968	12.910	54.596	1.00 23		В
25	MOTA	1790	CB	SER	240	25.778	13.249	55.480	1.00 22	. 32	В
	MOTA	1791	OG	SER	240	25.932	12.724	56.786	1.00 21	.48	В
	ATOM	1792	С	SER	240	26.704	13.447	53.199	1.00 23	. 92	Ð
	ATOM	1793	0	SER	240	27.065	14.568	52.865	1.00 23	. 73	В
	ATOM	1794	N	VAL	241	26.067	12.622	52.382	1.00 25		В
30		1795		VAL	241	25.712	12.995	51.022	1.00 25		В
50	MOTA		CA								
	MOTA	1796	CB	VAL	241	26.654	12.349	49.985	1.00 26		В
	ATOM	1797		VAL	241	26.790	10.856	50.249	1.00 26		В
	MOTA	1798	CG2	VAL	241	26.118	12.595	48.579	1.00 26	.95	В
	ATOM	1799	С	VAL	241	24.293	12.513	50.787	1.00 25	. 56	·B
35	MOTA	·1800	0	VAL	241	24.013	11.321	50.856	1.00 25	. 33	В
	MOTA	1801	N	THR	242	23.391	13.454	50.536	1.00 26		В
	ATOM	1802	CA	THR	242	21.996	13.130	50.302	1.00 26		В
		1803		THR	242	21.091	13.997	51.182	1.00 26		В
	MOTA		CB								
40	MOTA	1804		THR	242	21.447	13.814	52.557	1.00 26		В
40	ATOM	1805		THR	242	19.628	13.612	50.995	1.00 28		В
	ATOM	1806	С	THR	242	21.656	13.352	48.832	1.00 27	. 35	B
	MOTA	1807	0	THR	242	22.126	14.311	48.217	1.00 26	. 21	В
	MOTA	1808	N	ILE	243	20.857	12.451	48.263	1.00 28	. 40	В
	MOTA	1809	CA	ILE	243	20.468	12.564	46.861	1.00 28	. 65	В
45	MOTA	1810	CB	ILE	243	21.048	11.407	46.017	1.00 28		B
.5	MOTA	1811		ILE	243	20.944	11.746	44.534	1.00 27		B
	MOTA	1812		ILE	243	22.526	11.156	46.392	1.00 29		В
	MOTA	1813		ILE	243	23.191	10.046	45.592	1.00 25		В
50	MOTA	1814	С	ILE	243	18.950	12.538	46.721	1.00 29		В
50	MOTA	1815	0	ILE	243	18.327	11.512	46.966	1.00 30	.63	В
	MOTA	1816	N	HIS	244	18.355	13.672	46.358	1.00 31	.77	В
	MOTA	1817	CA	HIS	244	16.908	13.744	46.158	1.00 32	. 56	В
	ATOM	1818	CB	HIS	244	16.354	15.175	46.421	1.00 33		В
	MOTA	1819	CG	HIS	244	16.323	15.570	47.864	1.00 34		В
55		1820						48.785			В
22	MOTA			HIS	244	15.331	15.500		1.00 35		
	MOTA	1821		HIS	244	17.405	16.132	48.511	1.00 36		В
	MOTA	1822		HIS	244	17.080	16.392	49.765	1.00 35	. 67	В
	MOTA	1823	NE2	HIS	244	15.827	16.018	49.958	1.00 35	.06	₿.
	ATOM	1824	С	HIS	244	16.700	13.383	44.693	1.00 33	.70	В
60	MOTA	1825	0	HIS	244	17.271	14.020	43.798	1.00 33	. 29	В
	ATOM	1826	-	MET	245		12.366		1.00 34		В
							11.910				
	MOTA	1827	CA	MET	245	15.654		43.087	1.00 34		В
	MOTA	1828	CB	MET	245	16.212	10.483	42.944	1.00 34		В
65	MOTA	1829	CG	MET	245	17.734	10.441	43.100	1.00 35		В
65	MOTA	1830	SD	MET	245	18.439	8.805	43.321	1.00 36		В
	MOTA	1831	CE	MET	245	18.009	8.537	45.032	1.00 32	. 87	В
	ATOM	1832	C	MET		14.203	11.985	42.628	1.00 34		В
	MOTA	1833	õ	MET	245	13.272	11.757	43.402	1.00 33		В
			N		246	14.026	12.313		1.00 35		В
70	MOTA	1834		LYS				41.352			
70	MOTA	1835	CA	LYS	246	12.700	12.449	40.769	1.00 36		В
	ATOM	1836	CB	LYS	246	12.280	13.947	40.750	1.00 38		В
	MOTA	1837	CG	LYS	246	10.919	14.227	40.117	1.00 43		В
	ATOM	1838	CD	LYS	246	10.702	15.729	39.856	1.00 45	.60	В

	>mov				346				1 00 40 45	В
	ATOM	1839	CE	LYS	246	10.795	16.556	41.148	1.00 48.45	В
	ATOM	1840	NZ	LYS	246	10.619	18.031	40.940	1.00 46.59	В
	MOTA	1841	C	LYS	246	12.654	11.889	39.353	1.00 36.70	В
5	ATOM	1842	0	LYS	246	13.324	12.387	38.452 39.166	1.00 36.63	В
,	MOTA	1843	N	GLU	247	11.864	10.841		1.00 37.12	В
	MOTA	1844	CA	GLU	247	11.706	10.240	37.854		В
	MOTA	1845	CB	GLU	247	12.209	8.806	37.866	1.00 37.24	В
	MOTA	1846	CC	GLU	247	11.710	7.990	39.036	1.00 37.73	В
10	MOTA	1847	CD	GLU	247	12.621	6.820	39.347	1.00 38.20 1.00 37.07	В
10	MOTA	1848		GLU	247	12.293	6.035	40.262		В
	MOTA	1849	OE2	GLU	247 247	13.670	6.692	38.677	1.00 38.76 1.00 36.40	В
	MOTA	1850	C	GLU		10.228	10.299	37.498	1.00 35.40	В
	ATOM	1851 1852	0	GLU	247 248	9.369	10.193	38.365	1.00 37.67	В
15	MOTA	1853	N	THR		9.940	10.498	36.219	1.00 37.07	В
13	MOTA		CA	THR	248	8.563	10.587	35.746	1.00 39.40	В
	MOTA	1854	CB	THR	248	8.344	11.889	34.920 35.693	1.00 40.65	В
	MOTA		. 0G1		248	8.754	13.025		1.00 40.08	В
	MOTA MOTA	1856		THR	248	6.877	12.050	34.543 34.863	1.00 39.45	В
20		1857	C O	THR THR	248 248	8.240	9.381 9.095	33.902	1.00 39.20	В
20	MOTA MOTA	1858 1859	N	THR	249	8.959 7.158	8.678	35.187	1.00 39.85	В
			CA	THR	249		7.515	34.407	1.00 40.93	В
	MOTA MOTA	1860 1861	CB	THR	249	6.751 5.642	6.728	35.119	1.00 41.31	В
				THR	249			35.119	1.00 40.33	В
25	MOTA MOTA	1862		THR	249	4.458	7.531 6.345	36.527	1.00 39.92	В
25		1863 1864		THR	249	6.078 6.233	7.952	33.039	1.00 41.94	В
	MOTA MOTA	1865	C O	THR	249	6.178	9.145	32.736	1.00 41.92	В
	MOTA	1866	N	ILE	250	5.857	6.979	32.736	1.00 43.64	В
	MOTA	1867	CA	ILE	250	5.343	7.253	30.875	1.00 43.57	В
30	ATOM	1868	CB	ILE	250	5.340	5.970	30.004	1.00 43.38	В
50	ATOM	1869		ILE	250	4.228	5.029	30.465	1.00 41.86	B
	MOTA	1870		ILE	250	5.173	6.343	28.510	1.00 41.89	В
	MOTA	1871		ILE	250	5.286	5.169	27.560	1.00 39.31	В
	MOTA	1872	C	ILE	250	3.922	7.805	30.983	1.00 44.06	B
35	ATOM	1873	ŏ	ILE	250	3.320	8.197	29.984	1.00 43.16	В
55	MOTA	1874	N	ASP	251	3.402	7.834	32.209	1.00 45.37	В
	MOTA	1875	CA	ASP	251	2.059	8.353	32.493	1.00 47.36	В
	MOTA	1876	CB	ASP	251	1.319	7.437	33.502	1.00 47.52	В
	ATOM	1877	CG	ASP	251	0.719	6.208	32.852	1.00 46.95	В
40	ATOM	1878		ASP	251	0.222	5.335	33.595	1.00 46.42	В
	ATOM	1879		ASP	251	0.735	6.121	31.606	1.00 46.77	B
	ATOM	1880	c	ASP	251	2.097	9.778	33.061	1.00 48.00	В
	ATOM	1881	ō	ASP	251	1.052	10.349	33.377	1.00 49.62	В
	ATOM	1882	N	GLY	252	3.297	10.339	33.195	1.00 48.57	В
45	MOTA	1883	CA	GLY	252	3.445	11.684	33.725	1.00 48.41	В
	MOTA	1884	C	GLY	252	3.519	11.749	35.243	1.00 49.25	В
	MOTA	1885	ō	GLY	252	3.592	12.839	35.823	1.00 48.30	В
	MOTA	1886	N	GLU	253	3.489	10.584	35.890	1.00 49.52	В
	MOTA	1887	CA	GLU	253	3.555	10.504	37.349	1.00 49.94	В
50	MOTA	1888	СВ	GLU	253	2.989	9.156	37.839	1.00 51.87	В
	MOTA	1889	CG	GLU	253	3.083	8.942	39.349	1.00 55.20	В
	MOTA	1890	CD	GLU	253	2.805	7.498	39.764	1.00 57.60	В
	MOTA	1891	OE1	GLU	253	2.837	7.204	40.981	1.00 58.27	В
	MOTA	1892	OE2	GLU	253	2.558	6.655	38.875	1.00 58.42	В
55	MOTA	1893	С	GLU	253	4.996	10.659	37.835	1.00 49.08	В
	ATOM	1894	0	GLU	253	5.948	10.301	37.136	1.00 47.88	В
	MOTA	1895	N	GLU	254	5.148	11.187	39.043	1.00 48.18	В
	MOTA	1896	CA	GLU	254	6.471	11.394	39.610	1.00 48.03	В
	MOTA	1897	CB	GLU	254	6.633	12.854	40.000	1.00 48.74	В
60	MOTA	1898	CG	GLU	254	6.950	13.761	38.827	1.00 51.39	В
	MOTA	1899	CD	GLU	254	6.866	15.232	39.193	1.00 53.81	В
	MOTA	1900		GLU	254	7.184	15.575	40.356	1.00 54.50	В
	MOTA	1901	OE2	GLU	254	6.493	16.043	38.313	1.00 54.20	В
	MOTA	1902	С	GLU	254	6.817	10.497	40.797	1.00 46.73	В
65	MOTA	1903	0	GLU	254	6.111	10.466	41.805	1.00 46.07	В
	MOTA	1904	N	LEU	255	7.918	9.763	40.651	1.00 45.44	В
	HOTA	1905	CA	LEU	255	8.416	8.869	41.689	1.00 43.34	В
	MOTA	1906	CB	LEU	255	8.880	7.522	41.069	1.00 42.70	В
	ATOM .	1907	CG	LEU	255	7.888	6.755	40.138	1.00 42.10	В
70	MOTA	1908		LEU	255	8.584	5.548	39.528	1.00 41.93	В
	ATOM	1909		LEU	255	6.658	6.322	40.919	1.00 42.42	В
	MOTA	1910	C	LEU	255	9.603	9.591	42.329	1.00 42.63	В
	MOTA	1911	0	LEU	255	10.599	9.886	41.662	1.00 40.70	В

	MOTA	1912	N	VAL	256	9.484	9.890	43.617	1.00 41.65	В
	MOTA	1913	CA	VAL	256	10.540	10.594	44.326	1.00 41.53	В
	MOTA	1914	СВ	VAL	256	9.994	11.865	45.040	1.00 42.73	В
	MOTA	1915		VAL	256	9.445	12.851	44.013	1.00 41.79	В
5	ATOM	1916	CG2		256	8.899	11.487	46.028	1.00 43.14	В
_	MOTA	1917	C	VAL	256	11.192	9.691	45.357	1.00 40.91	В
	MOTA	1918	0	VAL	256	10.516	9.123	46.216	1.00 42.52	В
	MOTA	1919	N	LYS	257	12.507	9.542	45.255	1.00 38.10	В
10	MOTA	1920	CA	LYS	257	13.237	8.718	46.200	1.00 35.97	В
10	MOTA	1921	CB	LYS	257	13.712	7.370	45.525	1.00 37.07	В
	MOTA	1922	CG	LYS	257	14.482	7.490	44.219	1.00 35.97	В
	MOTA	1923	CD	LYS	257	14.612	6.108	43.592	1.00 34.96	В
	MOTA	1924	CE	LYS	257	15.566	6.085	42.412	1.00 36.06	В
	MOTA	1925	NZ	LYS	257	15.142	6.972	41.303	1.00 38.19	В
15	MOTA	1926	¢	LYS	257	14.408	9.497	46.777	1.00 34.33	В
	ATOM	1927	0	LYS	257	15.100	10.227	46.074	1.00 35.94	В
	MOTA	1928	N	ILE	258	14.618	9.345	48.074	1.00 31.24	В
	MOTA	1929	CA	ILE	258	15.677	10.066	48.747	1.00 27.10	В
	ATOM	1930	CB	ILE	258	15.077	10.988	49.842	1.00 28.34	В
20	MOTA	1931		ILE	258	16.181	11.791	50.516	1.00 26.47	В
	ATOM	1932		ILE	258	14.021	11.949	49.203	1.00 27.71	В
	ATOM	1933		ILE	258	13.168	12.703	50.214	1.00 25.91	В.
	ATOM	1934	c	ILE	258	16.695	9.136	49.382	1.00 24.38	В.
	ATOM	1935	ò	ILE	258	16.386	8.400	50.314	1.00 22.26	В
25										
LJ	MOTA	1936	N	GLY	259	17.917	9.182	48.872	1.00 22.97	В
	ATOM	1937	CA	GLY	259	18.975	8.359	49.422	1.00 22.93	В
	MOTA	1938	C	GLY	259	20.055	9.163	50.135	1.00 22.70	В
	MOTA	1939	0	GLY	259	20.561	10.161	49.609	1.00 21.85	В
20	MOTA	1940	N	LYS	260	20.410	8.731	51.339	1.00 21.39	В
30	MOTA	1941	CA	LYS	260	21.441	9.412	52.112	1.00 21.77	В
	MOTA	1942	CB	LYS	260	20.834	10.042	53.411	1.00 20.00	В
	MOTA	1943	CG	LYS	260	21.805	10.848	54.262	1.00 17.18	В
	MOTA	1944	CD	LYS	260	21.119	11.342	55.534	1.00 16.09	В
25	MOTA	1945	CE	LYS	260	22.049	12.181	56.417	1.00 16.97	В
35	ATOM	-1946	NZ	LYS	260	21.341	12.724	57.641	1.00 15.85	В
	ATOM	1947	C	LYS	260	22.545	8.419	52.469	1.00 21.92	В
	MOTA	1948	0	LYS	260	22.284	7.303	52.93B	1.00 22.32	В
	MOTA	1949	N	LEU	261	23.780	8.837	52.236	1.00 19.52	В
	MOTA	1950	CA	LEU	261	24.932	8.009	52.520	1.00 17.05	В
40	MOTA	1951	CB	LEU	261	25.693	7.741	51.235	1.00 14.85	. В
	ATOM	1952	CG	LEU	261	27.111	7.236	51.385	1.00 14.96	. в
	ATOM	1953		LEU	261	27.114	5.939	52.165	1.00 12.47	В
	MOTA	1954		LEU	261	27.730	7.054	50.019	1.00 12.11	В
	ATOM	1955	c	LEU	261	25.828	8.720	53.519	1.00 17.96	В
45	ATOM	1956	ō	LEU	261	26.258	9.850	53.284	1.00 16.25	В
	ATOM	1957	N	ASN	262	26.099	8.063	54.643	1.00 18.12	В
	MOTA	1958	CA	ASN	262	26.970	8.640	55.670	1.00 18.04	
										В
	MOTA	1959	CB	ASN	262	26.336	8.512	57.080	1.00 15.45	В
50	MOTA	1960	CG.	ASN	262	24.943	9.103	57.152	1.00 17.34	В
50	MOTA	1961		ASN	262	23.957	8.381	57.282	1.00 17.52	В
	MOTA	1962		ASN	262	24.855	10.420	57.070	1.00 17.02	В
	MOTA	1963	С	ASN	262	28.327	7.929	55.664	1.00 18.26	В
	MOTA	1964	0	ASN	262	28.399	6.697	-55.735	1.00 16.87	B
55	MOTA	1965	N	LEU	263	29.394	8.717	55.564	1.00 18.04	В
55	ATOM	1966	CA	LEU	263	30.759	8.200	55.560	1.00 17.90	В
	MOTA	1967	CB	LEU	263	31.482	8.723	54.339	1.00 15.70	В
	MOTA	1968	CG	LEU	263	30.717	B.283	53.075	1.00 17.05	В
	ATOM	1969	CD1	LEU	263	31.255	8.961	51.853	1.00 16.38	В
	MOTA	1970	CD2	LEU	263	30.812	6.754	52.929	1.00 18.46	В
60	MOTA	1971	С	LEU	263	31.411	8.688	56.849	1.00 18.79	В
	ATOM	1972	0	LEU	263	31.712	9.873	56.992	1.00 20.38	В
	ATOM	1973	N	VAL	264	31.614	7.774	57.794	1.00 18.49	В
	ATOM	1974	CA	VAL	264	32.183	8.128	59.093	1.00 18.30	В
	ATOM	1975	СB	VAL	264	31.335	7.529	60.228	1.00 18.68	В
65	MOTA	1976		VAL	264	31.752	8.115	61.561	1.00 17.56	В
	ATOM	1977		VAL		29.858				
					264		7.772	59.955	1.00 21.14	В
	ATOM	1978	C	VAL	264	33.627	7.696	59.333	1.00 19.31	В
	MOTA	1979	0	VAL	264	33.952	6.513	59.210	1.00 19.80	В
70	MOTA	1980	N	ASP	265	34.478	8.667	59.680	1.00 17.61	В
70	ATOM	1981	CA	ASP	265	35.880	8.419	59.995	1.00 15.36	В
	MOTA	1982	CB	ASP	265	36.771	9.484	59.355	1.00 14.42	В
	MOTA	1983	CC	ASP	265	38.258	9.279	59.658	1.00 16.29	В
	MOTA	1984	OD1	ASP	265	38.583	8.741	60.736	1.00 19.48	В

	MOTA	1985	002	ASP	265	39.110	9.677	58.832	1.00 16.17	В
	MOTA	1986	С	ASP	265	35.971	8.507	61.528	1.00 15.62	В
	ATOM	1987	0	ASP	265	36.119	9.593	62.086	1.00 17.19	В
	ATOM	1988	N	LEU	266	35.891	7.367	62.205	1.00 13.53	В
5										
,	ATOM	1989	CA	LEU	266	35.930	7.357	63.666	1.00 12.99	В
	ATOM	1990	CB	LEU	266	35.555	5.913	64.239	1.00 9.90	В
	ATOM	1991	CG	LEU	266	34.172	5.339	63.898	1.00 12.88	В
	MOTA	1992		LEU	266	34.070	3.881	64.374	1.00 12.44	В
	ATOM	1993	CD2	LEU	266	33.088	6.185	64.542	1.00 11.19	B
10	ATOM	1994	С	LEU	266	37.277	7.783	64.240	1.00 11.25	В
	ATOM	1995	0	LEU	266	38.274	7.867	63.532	1.00 7.77	В
	MOTA	1996	N	ALA	267	37.263	8.059	65.539	1.00 10.58	₿
	ATOM	1997	CA	ALA	267	38.453	8.422	66.284	1.00 13.04	В
								67.634		
15	MOTA	1998	СВ	ALA	267	38.057	9.029		1.00 11.27	В
15	MOTA	1999	С	ALA	267	39.221	7.125	66.507	1.00 14.13	В
	ATOM	2000	0	ALA	267	38.610	6.077	66.718	1.00 16.34	В
	ATOM	2001	N	GLY	268	40.546	7.190	66.475	1.00 14.85	В
	MOTA	2002	CA	GLY	268	41.347	5.999	66.688	1.00 17.83	В
	ATOM	2003	С	GLY	268	40.934	5.198	67.909	1.00 20.15	В
20	MOTA	2004	0	GLY	268	40.663	5.760	68.978	1.00 21.52	В
	MOTA	2005	N	SER	269	40.918	3.878	67.773	1.00 20.60	B
	MOTA	2006	CA	SER	269	40.500	3.017	68.878	1.00 23.05	В
	MOTA	2007	CB	SER	269	39.929	1.721	68.324	1.00 20.23	В
	ATOM	2008	OG	SER	269	40.842	1.099	67.442	1.00 17.43	В
25										
25	ATOM	2009	С	SER	269	41.546	2.678	69.941	1.00 26.49	В
	ATOM	2010	0	SER	269	41.227	1.969	70.903	1.00 27.04	В
	ATOM	2011	N	GLU	270	42.775	3.171	69.781	1.00 29.47	В
	MOTA	2012	CA	GLU	270	43.848	2.887	70.743	1.00 32.95	В
	ATOM	2013	CB	GLU	270	45.234	3.432	70.210	1.00 32.65	В
30	ATOM	2014	CG	GLU	270	45.405	4.968	70.193	1.00 30.27	В
-		2015								
	MOTA		CD	GLU	270	44.822	5.656	68.963	1.00 30.89	В
	MOTA	2016	OE1	GLU	270	44.879	6.908	68.911	1.00 32.19	₿
	MOTA	2017	OE2	GLU	270 .	44.315	4.961	68.052	1.00 28.80	В
	ATOM	201B	C	GLU	270	43.560	3.472	72.129	1.00 36.87	
35										В
22	MOTA	2019	0	CLU	270	43.380	4.681	72.277	1.00 39.21	В
	MOTA	2020	N	ASN	271	43.503	2.613	73.143	1.00 40.27	В
	ATOM	2021	CA	ASN	271	43.238	3.062	74.515	1.00 42.68	В
	MOTA	2022	CB	ASN	271	42.196	2.131	75.222	1.00 43.15	В
	ATOM	2023	CG	ASN	271	40.798	2.244	74.621	1.00 45.39	В
40	MOTA	2024	001	ASN	271	40.230	3.337	74.540	1.00 46.39	В
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	MOTA	2025		asn	271	40.232	1.109	74.210	1.00 43.39	B
	ATOM	2026	С	ASN	271	44.528	3.093	75.331	1.00 43.55	В
	ATOM	2027	0	ASN	271	45.603	2.746	74.833	1.00 43.93	В
	ATOM	2028	N	ASN	287	41.588	11.864	79.666	1.00 44.94	В
45										
40	ATOM	2029	CA	ASN	287	40.716	12.252	78.558	1.00 45.22	В
	ATOM	2030	CB	ASN	287	41.514	13.086	77.476	1.00 48.29	В
	MOTA	2031	CG	ASN	287	42.261	14.276	78.074	1.00 50.68	В
	MOTA	2032		ASN	287	43.249	14.106	78.796	1.00 51.76	B
	MOTA	2033	NDZ	asn	287	41.791	15.488	77.774	1.00 51.75	В
50	ATOM	2034	С	ASN	287	40.091	11.016	77.897	1.00 42.90	В
	MOTA	2035	ō	ASN	287	40.787	10.182	77.315	1.00 42.06	В
	MOTA	2036	N	ILE	288	38.771	10.914	77.995	1.00 40.12	В
	MOTA	·2037	CA	ILE	288	38.034	9.794	77.424	1.00 36.62	В
	MOTA	2038	CB	ILE	288	37.110	9.146	78.479	1.00 37.65	В
55										
23	MOTA	2039		ILE	288	37.911	8.154	79.325	1.00 38.70	В
	MOTA	2040	CG1	ILE	288	36.464	10.252	79.390	1.00 36.64	В
	MOTA	2041	CD1	ILE	288	35.583	11.252	78.657	1.00 36.28	В
	MOTA	2042	C	ILE	288	37.183	10.200	76.230	1.00 33.35	В
~	MOTA	2043	0	ILE	288	36.763	11.356	76.100	1.00 34.53	В
60	MOTA	2044	N	ASN	289	36.938	9.252	75.342	1.00 27.16	В
	MOTA	2045	CA	ASN	289	36.112	9.564	74.199	1.00 23.25	В
	MOTA	2046	CB	ASN	289	36.731	9.052	72.954	1.00 20.82	B
	MOTA	2047	CG	ASN	289	36.172	9.721	71.712	1.00 19.85	В
	ATOM	2048	OD1		289	36.929	10.208	70.878	1.00 19.66	В
65										
00	ATOM	2049	ND2		289	34.846	9.737	71.576	1.00 17.37	В
	MOTA	2050	С	ASN:	289	34.763	8.912	74.459	1.00 20.79	В
	MOTA	2051	0	ASN	289	34.553	7.735	74.170	1.00 18.65	B
	MOTA	2052	N	GLN	290	33.863	9.694	75.042	1.00 19.57	В
70	MOTA	2053	CA	GLN	290	32.537	9.216	75.379	1.00 19.29	В
70	MOTA	2054	СĖ	GLN	290	31.678	10.366	75.901	1.00 19.26	В
	MOTA	2055	CG							
				GLN	290	30.278	9.942	76.312	1.00 19.65	В
	MOTA	2056	CD	GLN	290	30.265	8.891	77.423	1.00 20.79	В
	ATOM	2057	OE1		290	29.211	8.339	77.754	1.00 21.88	B
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	MOTA	2058	ME 2	GLN	290	21 427	0 (01	78.006	1 00 10 10	
						31.427	8.621		1.00 18.18	В
	MOTA	2059	С	GLN	290	31.830	8.538	74.214	1.00 18.80	В
	MOTA	2060	0	GLN	290	31.199	7.502	74.397	1.00 17.47	В
	ATOM	2061	N	SER	291	31.939	9.122	73.021	1.00 18.97	В
5	MOTA	2062	CA	SER	291	31.289		71.841	1.00 18.84	В
-							8.565			
	ATOM	2063	CB	SER	291	31.326	9.565	70.646	1.00 19.15	В
	MOTA	2064	OG	SER	291	30.347	10.593	70.784	1.00 19.00	В
	MOTA	2065	С	SER	291	31.897	7.239	71.420	1.00 19.68	В
	ATOM	2066	ō	SER	291	31.173	6.323	71.027	1.00 21.26	В
10										
10	ATOM	2067	N	LEU	292	33.219	7.131	71.494	1.00 18.43	В
	MOTA	2068	CA	LEU	292	33.872	5.888	71.128	1.00 17.73	В
	MOTA	2069	CB	LEU	292	35.361	6.070	71.140	1.00 15.77	В
	MOTA	2070	CG	LEU	292	36.119	4.969	70.418	1.00 15.31	В
15	ATOM	2071	CD1		292	35.703	4.951	68.953	1.00 11.07	В
15	ATOM	2072	CD2	LEU	292	37.621	5.213	70.548	1.00 16.30	В
	MOTA	2073	С	LEU	292	33.461	4.827	72.159	1.00 19.37	В
	MOTA	2074	٥	LEU	292	33.107	3.698	71.814	1.00 20.03	В
		2075	N		293					
	ATOM			LEU		33.504	5.219	73.430	1.00 19.01	В
20	MOTA	2076	CA	LEU	293	33.137	4.357	74.531	1.00 18.18	В
20	ATOM	2077	CB	LEU	293	33.194	5.140	75.819	1.00 16.50	В
	ATOM	2078	CG	LEU	293	34.193	4.752	76.903	1.00 18.80	В
	ATOM	2079		LEU	293	35.291	3.824	76.354	1.00 14.59	В
										•
	ATOM	2080	CD2		293	34.789	6.039	77.485	1.00 18.33	В
~-	MOTA	2081	С	LEU	293	31.724	3.828	74.326	1.00 20.79	В
25	ATOM	2082	0	LEU	293	31.446	2.629	74.480	1.00 21.79	В
	ATOM	2083	N	THR	294	30.824	4.730	73.972	1.00 20.82	В
	MOTA	2084	CA	THR		29.444	4.348	73.785	1.00 21.70	В
	MOTA	2085	CB	THR	294	28.556	5.607	73.770	1.00 21.45	В
	ATOM	2086	0G1	THR	294	28.737	. 6.305	75.012	1.00 20.05	В
30	MOTA	2087	CG2		294	27.085	5.243	73.638	1.00 23.08	В
	ATOM	2088	С	THR	294	29.245	3.488	72.541	1.00 22.57	В
	ATOM	2089	0	THR	294	28.410	2.589	72.541	1.00 24.83	В
	ATOM	2090	N	LEU	295	30.028	3.726	71.492	1.00 22.48	В
	MOTA	2091	CA	LEU	295	29.888	2.929	70.278	1.00 20.67	В
35	ATOM									
23		-2092	CB	LEU	295	30.896	3.354	69.239	1.00 16.50	В
	MOTA	2093	CG	LEU	295	30.872	2.542	67.933	1.00 15.31	В
	MOTA	2094	CD1	LEU	295	29.480	2.540	67.301	1.00 9.83	В
	MOTA	2095	CD2	LEU	295	31.901	3.126	66.996	1.00 13.69	В
	ATOM	2096	c	LEU	295					
40						30.072	1.453	70.614	1.00 21.75	В
40	MOTA	2097	0	LEU	295	29.261	0.620	70.222	1.00 22.82	B
	ATOM	2098	N	GLY	296	31.141	1.141	71.345	1.00 22.87	В
	MOTA	2099	CA	GLY	296	31.402	-0.230	71.753	1.00 21.35	В
	ATOM	2100	C	GLY	296	30.318	-0.785	72.668	1.00 20.58	В
45	ATOM	2101	0	GLY	296	29.960	-1.950	72.566	1.00 22.84	В
43	MOTA	2102	N	ARG	297	29.782	0.034	73.562	1.00 19.00	В
	MOTA	2103	CA	ARG	297	28.735	-0.441	74.462	1.00 18.91	В
	MOTA	2104	CB	ARG	297	28.530	0.539	75.601	1.00 17.91	В
	ATOM	2105	CG	ARG	297	29.645	0.523	76.596	1.00 17.55	В
50	MOTA	2106	CD	ARG	297	29.622	1.775	77.433	1.00 21.12	В
20	MOTA	2107	NE	ARG	297	30.783	1.860	78.311	1.00 20.84	В
	MOTA	2108	CZ	ARG	297	31.212	2.987	78.862	1.00 19.95	В
	MOTA	2109	NH1	ARG	297	30.567	4.118	78.614	1.00 19.89	В
	ATOM	2110	NH2		297	32.274	2.982	79.661	1.00 15.55	В
55	ATOM	2111	Ç	ARG	297	27.419	-0.662	73.733	1.00 18.05	В
55	ATOM	2112	0	ARG	297	26.581	-1.440	74.177	1.00 18.18	В
	ATOM	2113	N	VAL	298	27.235	0.035	72.618	1.00 19.06	В
	MOTA	2114	CA	VAL	298	26.019	-0.106	71.823	1.00 17.97	B
	MOTA	2115	CB	VAL	298	25.816	1.111	70.885	1.00 15.95	B
	MOTA	2116	CG1	VAL	298	24.691	0.843	69.899	1.00 13.08	В
60	ATOM	2117	CG2	VAL	298	25.507	2.350	71.710	1.00 14.44	В
	MOTA	2118	С	VAL	298	26.140	-1.377			В
				VAL				70.985	1.00 19.67	
	ATOM	2119	0		298	25.153	-2.075	70.749	1.00 21.91	В
	MOTA	2120	N	ILE	299	27.356	-1.686	70.544	1.00 19.47	В
	MOTA	2121	CA	ILE	299	27.570	-2.879	69.736	1.00 21.25	В
65	MOTA	2122	CB	ILE	299	28.973	-2.830	69.068	1.00 21.35	В
	ATOM	2123		ILE	299	29.354				
							-4.192	68.502	1.00 19.14	В
	MOTA	2124		ILE	299	28.950	-1.752	67.932	1.00 19.67	В
	MOTA	2125	CD1	ILE	299	30.316	-1.238	67.523	1.00 19.64	В
	MOTA	2126	C	ILE	299	27.399	-4.122	70.610	1.00 22.50	В
70	ATOM	2127	ŏ	ILE	299	26.774	-5.102	70.206		
, 5									1.00 21.52	В
	MOTA	2128	N	THR	300	27.936	-4.057	71.821	1.00 23.04	В
	ATOM	2129	CA	THR	300	27.827	-5.153	72.763	1.00 23.72	В
	MOTA	2130	CB	THR	300	28.521	-4.787	74.068	1.00 23.18	В
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	MOTA	2131	0G1	THR	300	29.923	-4.646	73.811	1.00 21.92	В
	MOTA	2132	CG2	THR	300	28.284	-5.841	75.138	1.00 17.93	B
	MOTA	2133	C	THR	300	26.353	-5.447	73.020	1.00 27.59	В
	MOTA	2134	0	THR	300	25.878	-6.563	72.787	1.00 27.46	В
5	MOTA	2135	N	ALA	301	25.626	-4.438	73.480	1.00 29.03	B
•	HOTA	2136	CA	ALA	301	24.206	-4.600	73.754	1.00 30.76	В
	ATOM	2137	СВ	ALA	301	23.598	-3.262	74.139	1.00 31.16	В
	ATOM	2138	C	ALA	301	23.437	-5.196	72.573	1.00 32.99	В
		2139	o			22.545				
10	MOTA			ALA	301			72.772	1.00 35.01	В
10	ATOM	2140	N	LEU	302	23.770	-4.780	71.351	1.00 34.50	В
	MOTA	2141	CA	LEU	302	23.088	-5.279	70.152	1.00 34.70	В
	MOTA	2142	СВ	LEU	302	23.440	-4.425	68.943	1.00 35.01	В
	MOTA	2143	CG	LEU	302	22.840	-2.999	68.895	1.00 35.55	B
	ATOM	2144	CD1	LEU	302	23.474	-2.227	67.759	1.00 36.40	Ð
15	ATOM	2145	CD2	LEU	302	21.334	-3.063	68.714	1.00 33.89	В
	MOTA	2146	С	LEU	302	23.451	-6.721	69.855	1.00 35.87	В
	MOTA	2147	0	LEU	302	22.590	-7.547	69.549	1.00 36.50	В
•	MOTA	2148	N	VAL	303	24.742	-7.008	69.941	1.00 36.97	В
	ATOM	2149	CA	VAL	303	25.271	-8.339	69.691	1.00 36.81	В
20	ATOM	2150	СВ	VAL	303	26.818	-8.289	69.707	1.00 36.26	В
	MOTA	2151	CG1	VAL	303	27.402	-9.658	69.961	1.00 35.12	В
	ATOM	2152	CG2		303	27.316	-7.726	68.384	1.00 35.06	В
	MOTA	2153	c	VAL	303	24.757	-9.359	70.711	1.00 38.19	В
	MOTA	2154	ō	VAL	303		-10.506	70.368	1.00 39.57	В
25						24.495				
23	MOTA	2155	N	GLU	304	24.597	-8.928	71.957	1.00 39.43	В
	MOTA	2156	CA	GLU	304	24.129	-9.796	73.032	1.00 40.38	8
	MOTA	2157	CB	GLU	304	24.768	-9.359	74.350	1.00 41.03	В
	MOTA	2158	CG	GLU	304	26.290	-9.464	74.347	1.00 42.14	В
20	MOTA	2159	ന	GLU	304	26.889	-9.210	75.713	1.00 43.89	В
30	ATOM	2160	OE1		304	28.116	-9.390	75.879	1.00 42.77	В
	MOTA	2161	OE2		.304	26.127	-8.827	76.625	1.00 45.66	В
	MOTA	2162	С	GLU	304	22.612	-9.817	73.179	1.00 41.20	₿
	MOTA	2163	0	GLU	304	22.071	-10.477	74.062	1.00 39.68	В
25	MOTA	2164	N	ARG	305	21.932	-9.088	72.305	1.00 44.11	В
35	ATOM	2165	CA	ARG	305	20.474	-9.004	72.310	1.00 46.91	В
	ATOM	2166	CB	ARG	305	19.835	-10.408	71.997	1.00 48.72	В
	MOTA	2167	CG	ARG	305	20.520	-11.222	70.B97	1.00 52.86	В
	ATOM	2168	CD	ARG	305	20.686	-10.461	69.579	1.00 56.32	В
	ATOM	2169	NE	ARG	305	21.395	-11.268	68.582	1.00 59.70	В
40	ATOM	2170	CZ	ARG	305	21.970	-10.782	67.483	1.00 61.81	В
	MOTA	2171	NH1	ARG	305	21.926	-9.479	67.221	1.00 61.95	В
	MOTA	2172	NH2	ARG	305	22.605	-11.601	66.649	1.00 61.81	В
	MOTA	2173	С	ARG	305	19.890	-8.469	73.620	1.00 47.13	В
	MOTA	2174	0	ARG	305	18.784	-8.840	73.996	1.00 48.14	В
45	MOTA	2175	N	THR	306	20.621	-7.599	74.311	1.00 48.36	В
	ATOM	2176	CA	THR	306	20.135	-7.027	75.568	1.00 49.45	В
	MOTA	2177	CB	THR	306	21.275	-6.367	76.356	1.00 49.08	В
	MOTA	2178		THR	306	22.429	-7.214	76.326	1.00 49.36	В
	MOTA	2179		THR	306	20.862	-6.155	77.802	1.00 48.92	В
50	MOTA	2180	C	THR	306	19.066	-5.972	75.262	1.00 50.64	В
	ATOM	2181	ŏ	THR	306	19.275	-5.091	74.428	1.00 51.81	В
	ATOM	2182	N	PRO	307	17.910	-6.044	75.942	1.00 51.76	В
	ATOM	2183	CD	PRO	307	17.651	-6.959	77.06B	1.00 52.91	В
									1.00 52.91	
55	ATOM ATOM	2184	CA.	PRO	307 307	16.779	-5.119	75.761		В
J.J		2185	CB	PRO		15.945	-5.358	76.995	1.00 52.53	В
	MOTA	2186	CG	PRO	307	16.158	-6.818	77.257	1.00 53.28	В
	ATOM	2187	C	PRO	307	17.124	-3.638	75.585	1.00 51.42	В
	ATOM	2188	0	PRO	307	16.624	-2.983	74.664	1.00 51.33	В
۷۸	MOTA	2189	N	HIS	308	17.973	-3.115	76.466	1.00 49.88	В
60	MOTA	2190	CA	HIS	308	18.359	-1.711	76.410	1.00 47.29	В
	ATOM	2191	CB	HIS	308	18.432	-1.141	77.832	1.00 50.27	В
	MOTA	2192	CG	HIS	308	18.812	0.306	77.877	1.00 54.50	В
	ATOM	2193	CD2	HIS	308	19.992	0.909	78.158	1.00 55.48	В
	MOTA	2194		HIS	308	17.931	1.318	77.559	1.00 55.94	В
65	ATOM	2195		HIS	308	18.552	2.482	77.641	1.00 56.20	В
	ATOM	2196		HIS	308	19.804	2.262	78.003	1.00 56.35	В
	ATOM	2197	c	HIS	308	19.685	-1.445	75.690	1.00 43.71	В
	ATOM	2198	ō	HIS	308	20.709	-2.061	75.991	1.00 43.17	В
	MOTA	2199	N	VAL	309	19.649	-0.517	74.737	1.00 39.63	В
70	ATOM	2200	CA	VAL	309	20.829	-0.117	73.964	1.00 34.96	В
. •	ATOM	2201	CB	VAL	309	20.561	-0.206	72.449	1.00 34.96	В
	MOTA	2202		VAL	309	21.858	0.013			
								71.675	1.00 34.27	В
	MOTA	2203	C02	VAL	309	19.934	-1.548	72.114	1.00 32.68	В

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	ATOM	2204	С	VAL	309	21.086	1.344	74.336	1.00 31.77	В
	ATOM	2205	0	VAL	309	20.237	2.204	74.102	1.00 30.77	В
	ATOM	2206	N	PRO	310	22.266	1.642	74.906	1.00 29.55	В
_	ATOM	2207	CD	PRO	310	23.347	0.670	75.171	1.00 27.65	В
5	ATOM	220B	CA	PRO	310	22.652	2.997	75.335	1.00 29.03	В
	ATOM	2209	CB	PRO	310	23.856	2.732	76.230	1.00 29.20	В
		. 2210	CG	PRO	310	24.518	1.555	75.539	1.00 27.40	В
	ATOM	2211	c	PRO	310	22.949	4.064	74.268	1.00 28.13	В
		2212	ō	PRO	310	23.960	4.760	74.357	1.00 27.93	В
10	ATOM					22.064			1.00 27.73	В
10	MOTA	2213	N	TYR	311		4.198	73.284		
	MOTA	2214	CA	TYR	311	22.217	5.175	72.203	1.00 28.46	В
	MOTA	2215	CB	TYR	311	20.949	5.195	71.291	1.00 29.00	В
	MOTA	2216	CG	TYR	311	20.724	3.960	70.450	1.00 32.30	В
1.5	MOTA	2217	CD1	TYR	311	21.600	3.631	69.413	1.00 32.05	В
. 15	MOTA	2218	CE1	TYR	311	21.393	2.492	68.628	1.00 34.37	В
	MOTA	2219	CD2	TYR	311	19.627	3.119	70.686	1.00 31.31	В
	ATOM	2220	CE2	TYR	311	19.411	1.979	69.908	1.00 32.07	В
	ATOM	2221	CZ	TYR	311	20.299	1.669	68.882	1.00 34.42	В
	MOTA	2222	ОН	TYR	311	20.120	0.531	68.122	1.00 35.43	В
20	ATOM	2223	С	TYR	311	22.458	6.611	72.678	1.00 28.67	В
	ATOM	2224	0	TYR	311	23.343	7.296	72.177	1.00 27.07	В
	ATOM	2225	N	ARG	312	21.652	7.059	73.635	1.00 29.15	В
	MOTA	2226	CA	ARG	312	21.716	8.425	74.143	1.00 29.95	В.
	MOTA	2227	CB	ARG	312	20.481	8.724	74.961	1.00 32.31	В
25	ATOM	2228	CG	ARG	312	19.189	8.626	74.196	1.00 36.65	В
25								75.169	1.00 40.81	В
	MOTA	2229	CD	ARG	312	18.046	8.529			
	MOTA	2230	NE	ARG	312	16.862	7.919	74.577	1.00 43.18	В
	ATOM	2231	CZ	ARG	312	15.951	7.251	75.278	1.00 45.73	В
20	MOTA	2232		ARG	312	16.100	7.108	76.597	1.00 44.15	В
30	MOTA	2233		ARG	312	14.888	6.737	74.664	1.00 45.91	В
	MOTA	2234	С	ARG	312	22.926	8.811	74.969	1.00 28.83	В
	MOTA	2235	0	ARG	312	23.104	9.991	75.276	1.00 29.69	В
	MOTA	2236	N	GLU	313	23.755	7.843	75.340	1.00 26.62	В
~ =	MOTA	2237	CA	GLU	313	24.917	8.160	76.153	1.00 22.31	В
35	ATOM	2238	CB	GLU	313	25.419	6.929	76.814	1.00 22.37	В
	MOTA	2239	CG	GLU	313	24.550	6.521	77.994	1.00 24.92	В
	MOTA	2240	CD	GLU	313	24.871	5.136	78.554	1.00 26.13	В
	MOTA	2241	OE1	GLU	313	26.060	4.823	78.755	1.00 27.91	В
	MOTA	2242	OE2	GLU	313	23.926	4.365	78.813	1.00 27.77	В
40	MOTA	2243	С	GLU	313	26.031	8.873	75.403	1.00 21.16	В
	MOTA	2244	0	GLU	313	27.096	9.122	75.963	1.00 21.76	В
	ATOM	2245	N	SER	314	25.789	9.222	74.144	1.00 18.52	В
	MOTA	2246	CA	SER	314	26.796	9.935	73.375	1.00 19.81	В
	MOTA	2247	CB	SER	314	27.966	8.992	72.968	1.00 20.10	В
45	ATOM	2248	OG	SER	314	27.731	8.382	71.710	1.00 19.29	В
	MOTA	2249	c	SER	314	26.206	10.583	72.130	1.00 20.60	В
	MOTA	2250	ō	SER	314	25.198	10.126	71.597	1.00 19.90	В
	ATOM	2251	N	LYS	315	26.854	11.654	71.676	1.00 20.92	В
	ATOM	2252	CA	LYS	315	26.412	12.395	70.504	1.00 20.48	В
50		2253	CB	LYS	315	27.264	13.689	70.329	1.00 20.26	В
,50	ATOM									В
	MOTA	2254	CG	LYS	315	27.318	14.572	71.556	1.00 19.73	
	MOTA	2255	CD	LYS	315	25.936	14.893	72.074	1.00 22.19	В
	MOTA	2256	CE	LYS	315	25.984	15.989	73.129	1.00 23.41	В
55	MOTA	2257	NZ	LYS	315	26.408	17.293	72.528	1.00 26.09	В
55	ATOM	2258	Ç	LYS	315	26.513	11.560	69.239	1.00 19.78	В
	MOTA	2259	0	LYS	315	25.626	11.614	68.373	1.00 20.29	В
	MOTA	2260	N	LEU	316	27.598	10.796	69.130	1.00 17.65	В
	MOTA	2261	CA	LEU	316	27.808	9.962	67.955	1.00 17.80	В
	MOTA	2262	CB	LEU	316	29.209	9.245	68.013	1.00 16.46	В
60	MOTA	2263	CG	LEU	316	29.602	8.339	66.775	1.00 15.01	B
	MOTA	2264	CD1	LEU	316	29.683	9.151	65.507	1.00 14.12	В
	MOTA	2265		LEU	316	30.937	7.695	67.030	1.00 17.53	В
	ATOM	2266	c	LEU	316	26.698	8.926	67.798	1.00 17.14	В
	ATOM	2267	ō	LEU	316	26.060	8.854	66.742	1.00 17.17	В
65	MOTA	2268	N	THR	317	26.462	8.137	68.844	1.00 17.69	В
55	ATOM	2269	CA	THR	317	25.439	7.106	68.777	1.00 17.03	В
										В
	MOTA	2270	CB	THR	317	25.525	6.124	69.966	1.00 21.44	
	MOTA	2271		THR	317	25.617	6.848	71.198	1.00 21.96	В
70	MOTA	2272		THR	317	26.743	5.206	69.804	1.00 21.41	В
70	ATOM	2273	C	THR	317	24.031	7.659	68.659	1.00 18.09	В
	MOTA	2274	0	THR	317	23.155	6.990	68.130	1.00 17.17	В
	MOTA	2275	N	ARG	318	23.800	8.877	69.134	1.00 19.16	В
	ATOM	2276	CA	ARG	318	22.469	9.460	68.986	1.00 20.49	В

	MOTA	2277	CB	ARG	318	22.283	10.654	69.927	1.00 22.85	В
-	MOTA	2278	CG	ARG	318	22.155	10.218	71.387	1.00 28.27	В
	ATOM	2279	CD	ARG	318	21.942	11.375	72.318	1.00 31.62	В
					318			71.788	1.00 39.60	В
5	MOTA	2280	NE	ARG		20.929	12.277			
J	MOTA	2281	CZ	ARG	318	20.361	13.261	72.479	1.00 40.99	В
	MOTA	2282	NH1	ARG	318	20.703	13.474	73.746	1.00 41.19	В
	MOTA	2283	NH2	ARG	318	19.454	14.034	71.894	1.00 41.05	В
	ATOM	2284	С	ARG	318	22.288	9.873	67.525	1.00 20.16	В
	MOTA	2285	ō	ARG	318	21.237	9.648	66.929	1.00 21.26	В
10								66.932	1.00 18.27	В
10	MOTA	2286	N	ILE	319	23.332	10.435			
	MOTA	2287	CA	ILE	319	23.255	10.843	65.539	1.00 18.18	В
	MOTA	2288	CB	ILE	319	24.505	11.665	65.132	1.00 17.80	В
	MOTA	2289	CG2	ILE	319	24.482	11.913	63.619	1.00 17.11	В
	MOTA	2290	CG1	ILE	319	24.561	13.006	65.928	1.00 17.07	В
15	MOTA	2291	CD1	ILE	319	25.901	13.727	65.838	1.00 14.30	В
	MOTA	2292	c	ILE	319	23.134	9.663	64.550	1.00 18.77	В
	MOTA				319		9.753	63.569	1.00 16.28	В
		2293	0	ILE		22.397				
	MOTA	2294	N	LEU	320	23.B60	8.571	64.808	1.00 18.72	В
	MOTA	2295	CA	LEU	320	23.874	7.415	63.905	1.00 18.52	В
20	HOTA	2296	CB	LEU	320	25.323	7.003	63.621	1.00 14.27	В
	MOTA	2297	CG	LEU	320	26.321	8.000	63.025	1.00 16.38	В
	ATOM	2298		LEU	320	27.707	7.354	63.017	1.00 13.61	В
	ATOM	2299		LEU	320	25.905	8.426	61.605	1.00 14.32	В
		2300		LEU	320	23.113	6.159	64.354	1.00 21.16	В
25	ATOM		C							
25	ATOM	2301	0	LEU	320	23.308	5.087	63.780	1.00 21.77	B
	MOTA	2302	N	GLN	321	22.249	6.277	65.357	1.00 22.79	В
	ATOM	2303	CA	GLN	321	21.519	5.114	65.848	1.00 25.68	В
	ATOM	2304	CB	GLN	321	20.531	5.524	66.954	1.00 28.52	В
	HOTA	2305	CG	GLN	321	19.448	6.490	66.535	1.00 32.15	В
30	ATOM	2306	CD	GLN	321	18.539	6.843	67.700	1.00 35.99	В
-	ATOM	2307		GLN	321	17.953	5.954	68.332	1.00 33.89	В
									1.00 36.73	В
	ATOM	2308		GLN	321	18.417	8.144	67.997		
	MOTA	2309	С	GLN	321	20.790	4.254	64.813	1.00 25.53	В
25	MOTA	2310	0	GLIN	321	20.625	3.056	65.029	1.00 25.73	В
35	HOTA	2311	N	ASP	322	20.353	4.837	63.701	1.00 26.46	В
•	ATOH	2312	CA	ASP	322	19.659	4.040	62.695	1.00 28.33	В
	MOTA	2313	CB	ASP	322	18.913	4.934	61.681	1.00 29.02	В
	ATOM	2314	CG	ASP	322	17.894	4.152	60.847	1.00 30.51	В
								59.604	1.00 31.51	В
40	ATOM	2315		ASP	322	17.880	4.308			
40	MOTA	2316		ASP	322	17.100	3.384	61.434	1.00 29.46	В
	MOTA	2317	C	ASP	322	20.661	3.152	61.959	1.00 29.44	В
	MOTA	2318	0	ASP	322	20.284	2.195	61.280	1.00 29.55	В
	HOTA	2319	N	SER	323	21.943	3.480	62.095	1.00 29.59	В
	MOTA	2320	CA	SER	323	22.999	2.705	61.458	1.00 28.78	В
45	MOTA	2321	CB	SER	323	24.172	3.594	61.165	1.00 27.31	В
15		2322	OG	SER	323	23.845	4.545	60.178	1.00 26.34	В
	MOTA									В
	MOTA	2323	C	SER	323	23.453	1.519	62.322	1.00 29.30	
	HOTA	2324	0	SER	323	24.234	0.687	61.875	1.00 2B.51	В
	MOTA	2325	N	LEU	324	22.967	1.445	63.558	1.00 30.19	В
50	MOTA	2326	CA	LEU	324	23.338	0.354	64.451	1.00 30.51	В
	ATOM	2327	CB	LEU	324	24.110	0.893	65.662	1.00 30.62	В
	ATOM	2328	CG	LEU	324	25.577	1.365	65.474	1.00 29.76	В
	ATOM	2329		LEU	324	25.670	2.412	64.401	1.00 31.76	В
				LEU				66.775	1.00 28.62	В
55	MOTA	2330			324	26.085	1.928			
<i>JJ</i>	MOTA	2331	C	LEU	324	22.113	-0.419	64.927	1.00 31.44	В
	MOTA	2332	0	LEU	324	21.611	-0.184	66.026	1.00 32.71	В
	MOTA	2333	N	GLY	325	21.642	-1.347	64.095	1.00 31.87	В
	MOTA	2334	CA	GLY	325	20.479	-2.148	64.444	1.00 30.03	В
	MOTA	2335	С	GLY	325	19.190	-1.440	64.082	1.00 29.89	В
60	MOTA	2336	ŏ	GLY	325	18.160	-1.636	64.727	1.00 29.38	В
00										В
	ATOM	2337	N	GLY	326	19.253	-0.614	63.042	1.00 29.59	
	MOTA	2338	CA	GLY	326	18.092	0.139	62.603	1.00 27.99	В
	MOTA	2339	С	GLY	326	17.706	-0.236	61.193	1.00 27.84	В
	MOTA	2340	0	GLY	326	17.896	-1.378	60.811	1.00 28.56	В
65	MOTA	2341	N	ARG	327	17.197	0.719	60.418	1.00 26.60	В
-	ATOM	2342	CA	ARG	327	16.763	0.456	59.046	1.00 27.36	В
	ATOM	2343	CB	ARG	327	15.451	1.234	58.745	1.00 30.55	В
								59.943	1.00 34.58	В
	MOTA	2344	CG	ARG	327	14.534	1.451			
70	MOTA	2345	CD	ARG	327	13.775	0.198	60.367	1.00 40.44	В
70	MOTA	2346	NE	ARG	327	12.359	0.271	60.014	1.00 43.41	В
	MOTA	2347	CZ	ARG	327	11.898	0.209	58.768	1.00 47.99	В
	ATOM	2348		ARG	327	12.741	0.071	57.751	1.00 49.86	В
	ATOM	2349		ARG	327	10.592	0.285	58.535	1.00 48.98	В
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	MOTA	2350	С	ARG	327	17.796	0.811	57.967	1.00 27.20	В
	ATOM	2351	0	ARG	327	17.521	0.680	56.775	1.00 27.07	В
	MOTA	2352	N	THR	328	18.977	1.257	58.379	1.00 26.89	В
5	MOTA	2353	CA	THR	328	20.028	1.646	57.441	1.00 25.49	В
5	MOTA	2354	CB	THR	328	20.870	2.813	58.024	1.00 27.20	В
	MOTA MOTA	2355		THR	328	20.024	3.944	58.252	1.00 29.46	В
	MOTA	2356 2357	C	THR THR	328 328	21.992 20.974	3.210 0.492	57.072 57.125	1.00 26.15 1.00 24.96	B B
	ATOM	2358	ō	THR	328		-0.346	57.984	1.00 24.98	В
10	ATOM	2359	N	ARG	329	21.465	0.431	55.890	1.00 23.74	. В
	MOTA	2360	CA	ARG	329	22.426	-0.610	55.543	1.00 24.57	В
	MOTA	2361	CB	ARG	329	22.551	-0.842	54.014	1.00 26.29	В
	MOTA	2362	CG	ARG	329	23.421	-2.071	53.721	1.00 31.07	В
15	ATOM	2363	CD	ARG	329	24.277	-1.980	52.461	1.00 34.15	В
.15	MOTA	2364	NE	ARG	329	23.590	-2.447	51.259	1.00 37.59	В
	MOTA	2365	CZ	ARG	329	24.217	-2.885	50.168	1.00 38.17	В
	MOTA MOTA	2366 2367		ARG	329 329	25.547 23.513	-2.923 -3.284	50.124	1.00 38.35	В
	MOTA	2368	C	ARG	329	23.761	-0.102	49.119 56.061	1.00 36.37 1.00 22.51	B B
20	MOTA	2369	ŏ	ARG	329	24.174	1.012	55.741	1.00 21.91	В
	MOTA	2370	N	THR	330	24.431	-0.919	56.856	1.00 21.40	В
	MOTA	2371	CA	THR	330	25.704	-0.529	57.433	1.00 21.18	В
	MOTA	2372	CB	THR	330	25.610	-0.435	58.971	1.00 20.58	· B
25	MOTA	2373	0G1		330	24.666	0.581	59.317	1.00 22.60	В
25	MOTA	2374		THR	330	26.962	-0.099	59.581	1.00 17.89	В
	MOTA	2375	C	THR	330	26.837	-1.471	57.085	1.00 21.32	В
	MOTA MOTA	2376 2377	O N	THR SER	330 331	26.673 28.002	-2.691 -0.872	57.001 56.902	1.00 19.41	B B
	ATOM	2378	CA	SER	331	29.200	-1.602	56.574	1.00 21.39	В
30	ATOM	2379	СВ	SER	331	29.469	-1.473	55.084	1.00 22.34	В
	ATOM	2380	0G	SER	331	30.537	-2.313	54.694	1.00 26.49	В
	MOTA	2381	С	SER	331	30.340	-1.001	57.391	1.00 20.49	В
	MOTA	2382	0	SER	331	30.418	0.208	57.565	1.00 21.48	В
35	MOTA	2383	N	ILE	332	31.213	-1.849	57.911	1.00 18.89	В
23	ATOM ATOM	2384	CA	ILE	332	32.341	-1.371	58.695	1.00 15.95	В
	ATOM	2385 2386	CB	ILE	332 332	32.321 33.621	-1.936 -1.568	60.135 60.854	1.00 15.17 1.00 12.52	B B
	ATOM	2387	_	ILE	332	31.091	-1.447	60.882	1.00 12.52	В
	ATOM	2388		ILE	332	30.932	-2.097	62.247	1.00 7.00	В
40	ATOM	2389	C	ILE	332	33.650	-1.818	58.063	1.00 15.41	В
	ATOM	2390	0	ILE	332	33.802	-2.980	57.687	1.00 12.48	В
	MOTA	2391	N	ILE	333	34.591	-0.088	57.948	1.00 16.21	В
	MOTA	2392	CA	ILE	333	35.899	-1.203	57.411	1.00 16.71	В
45	MOTA	2393	CB	ILE	333	36.310	-0.266	56.273	1.00 16.82	В
73	MOTA	2394 2395		ILE	333 333	37.616 35.242	-0.744 -0.259	55.675 55.169	1.00 15.94 1.00 16.68	B B
	ATOM	2396	CD1		333	35.557	0.705	54.012	1.00 15.18	В
	ATOM	2397	c	ILE	333	36.860	-1.021	58.561	1.00 18.56	В
	MOTA	2398	0	ILE	333	37.074	0.104	59.032	1.00 21.41	В
50	MOTA	2399	N	ALA	334	37.411	-2.137	59.035	1.00 20.14	В
	MOTA	2400	CA	ALA	334	38.360	-2.125	60.147	1.00 19.94	В
	MOTA	2401	СВ	ALA	334	38.182	-3.362	61.020	1.00 18.30	. В
	MOTA MOTA	2402 2403	С 0	ALA ALA	334	39.756	-2.096 -2.989	59.550 58.790	1.00 20.34	В
55	ATOM	2404	N	THR	334 335	40.135 40.514	-1.062	59.897	1.00 20.44	B
-	ATOM	2405	CA	THR	335	41.853	-0.901	59.369	1.00 19.70	В
	MOTA	2406	СВ	THR	335	42.106	0.584	59.008	1.00 21.15	В
	MOTA	2407	0G1	THR	335	41.876	1.409	60.157	1.00 24.31	В
~	MOTA	2408	CG2	THR	335	41.158	1.026	57.905	1.00 21.90	В
60	MOTA	2409	С	THR	335	42.907	-1.403	60.351	1.00 19.67	В
	ATOM	2410	0	THR	335		-1.190	61.559	1.00 20.81	В
	MOTA	2411	N	ILE	336	43.924	-2.085	59.833	1.00 19.06	В
	MOTA MOTA	2412 2413	CA	ILE	336	44.991	-2.618 -4.147	60.680	1.00 19.16	В
65	MOTA	2414	CB	ILE	336 336	44.845 43.519	-4.470	60.882 61.562	1.00 18.20 1.00 17.20	B B
	ATOM	2415		ILE	336	44.933	-4.857	59.564	1.00 15.56	В
	ATOM	2416		ILE	336	44.926	-6.371	59.697	1.00 16.09	В
	MOTA	2417	c	ILE	336	46.388	-2.343	60.116	1.00 19.85	В
70	MOTA	2418	0	ILE	336	46.547	-1.995	58.945	1.00 20.63	В
70	MOTA	2419	N	SER	337	47.395	-2.487	60.970	1.00 21.82	В
	MOTA	2420	CA	SER	337	48.788	-2.277	60.576	1.00 23.86	В
	MOTA	2421	CB	SER	337	49.514	-1.430	61.611	1.00 22.35	В
	MOTA	2422	0G	SER	337	50.551	-2.165	62.229	1.00 19.41	В

	ATOM	2423	C	SER	337	49.507	-3.622	60.458	1.00 26.10	В
	MOTA	2424	0	SER	337	49.133	-4.597	61.119	1.00 25.43	В
	MOTA	2425	N	PRO	338	50.543	-3.692	59.606	1.00 26.45	В
_. 5	MOTA	2426	CD	PRO	338	50.873	-2.755	58.518	1.00 26.43	В
	MOTA	2427	CA	PRO	338	51.287	-4.943	59.441	1.00 27.75	В
	MOTA	2428	CB	PRO	338	51.703	-4.893	58.009	1.00 25.91	В
	MOTA	2429 2430	cc	PRO	338	52.043	-3.453	57.835	1.00 26.04	В
	MOTA	2430	C	PRO	338	52.493 53.304	-5.016	60.366	1.00 28.99	В
10	MOTA MOTA	2431	N	PRO	338		-5.929	60.250	1.00 30.27	В
10	ATOM	2432	CA	ALA ALA	339 339	52.615 53.765	-4.057	61.280	1.00 29.91	В
	MOTA	2434	CB	ALA	339	54.076	-4.024 -2.582	62.184 62.598	1.00 31.92	B B
	ATOM	2435	C	ALA	339	53.576	-4.884	63.415	1.00 32.09	В
	ATOM	2436	Ö	ALA	339	52.483	-4.965	63.959	1.00 34.29	В
15	ATOM	2437	N	SER	340	54.651	-5.525	63.856	1.00 31.24	B
	ATOM	2438	CA	SER	340	54.580	-6.374	65.030	1.00 29.08	В
	ATOM	2439		SER	340	55.877	-7.280	65.138	1.00 29.57	В
	ATOM	2440	OG	SER	340	57.053	-6.513	65.327	1.00 28.10	В
	MOTA	2441	Ċ	SER	340	54.396	-5.555	66.307	1.00 28.00	В
20	MOTA	2442	0	SER	340	53.844	-6.046	67.280	1.00 28.20	В
	ATOM	2443	N	LEU	341	54.852	-4.308	66.309	1.00 28.24	В
	ATOM-	2444	CA	LEU	341	54.715	-3.471	67.493	1.00 28.05	В
	MOTA	2445	СВ	LEU	341	55.742	-2.306	67.463	1.00 29.43	В
	MOTA	2446	CG	LEU	341	55.315	-0.861	67.190	1.00 30.31	В
25	ATOM	2447	CD1	LEU	341	56.404	0.084	67.690	1.00 28.26	В
	MOTA	244B	CD2	LEU	341	55.065	-0.659	65.707	1.00 31.94	В
	MOTA	2449	C	LEU	341	53.290	-2.936	67.647	1.00 28.81	В
	ATOM	2450	0	LEU	341	52.954	-2.305	68.650	1.00 28.00	В
20	MOTA	2451	N	ASN	342	52.450	-3.209	66.656	1.00 28.88	В
30	ATOM	2452	CA	ASN	342	51.060	-2.780	66.690	1.00 29.97	В
	MOTA	2453	CB	ASN	342	50.689	-2.094	65.369	1.00 28.90	В
	MOTA	2454	CG	ASN	342	51.256	-0.680	65.258	1.00 29.29	В
	MOTA	2455		ASN	342	51.568	-0.210	64.161	1.00 27.68	В
25	MOTA	2456		ASN	342	51.373	0.007	66.394	1.00 26.96	В
35	MOTA	2457	С	ASN	342	50.185	-4.010	66.902	1.00 31.53	В
	MOTA	2458	0	ASN	342	48.958	-3.956	66.765	1.00 32.86	В
	MOTA	2459	N	LEU	343	50.830	-5.118	67.252	1.00 30.95	В
	MOTA	2460	CA	LEU	343	50.143	-6.387	67.474	1.00 30.40	В
40	ATOM	2461	CB	LEU	343	51.167	-7.448	67.961	1.00 31.48	В
40	MOTA	2462	CG	LEU	343	50.755	-8.930	68.109	1.00 33.60	В
	MOTA	2463		LEU	343	50.408	-9.217	69.553	1.00 34.09	В
	ATOM ATOM	2464 2465		LEU	343	49.599	-9.270	67.168	1.00 31.95	В
	MOTA	2466	0	LEU	343 343	48.945 47.839	-6.325 -6.698	68.422	1.00 28.19	В
45	MOTA	2467	N	GLU	344	49.145	-5.858	68.042 69.647	1.00 29.33	B B
	MOTA	2468	CA	GLU	344	48.035	-5.787	70.598	1.00 25.82	В
	MOTA	2469	СВ	GLU	344	48.537	-5.276	71.962	1.00 27.56	В
	MOTA	2470	CG	CLU	344	47.438	-4.776	72.879	1.00 33.02	В
	ATOM -	2471	CD	GLU	344	47.884	-4.708	74.329	1.00 36.74	В
50	ATOM	2472		GLU	344	49.011	-4.222	74.583	1.00 36.88	В
	MOTA	2473		GLU	344	47.104	-5.138	75.217	1.00 38.52	В
	MOTA	2474	С	GLU	344	46.843	-4.948	70.122	1.00 23.12	В
	MOTA	2475	0	GLU	344	45.696	-5.357	70.265	1.00 22.53	В
	MOTA	2476	N	GLU	345	47.102	-3.775	69.564	1.00 22.13	В
55	MOTA	2477	CA	GLU	345	46.007	-2.949	69.082	1.00 22.56	В
	MOTA	2478	CB	GLU	345	46.484	-1.487	68.830	1.00 23.16	В
	ATOM	2479	CG	GLU	345	46.722	-0.693	70.108	1.00 23.64	В
	MOTA	2480	CD	GLU	345	45.440	-0.386	70.872	1.00 25.85	В
60	MOTA	2481	0E1	GLU	345	45.530	0.135	72.003	1.00 29.18	В
60	MOTA	2482	OE2	GLU	345	44.342	-0.653	70.352	1.00 25.14	B
	MOTA	2483	С	GLU	345	45.422	-3.566	67.808	1.00 21.03	B
	MOTA	2484	0	GLU	345	44.238	-3.398	67.519	1.00 20.99	В
	MOTA	2485	N	THR	346	46.253	-4.274	67.048	1.00 20.57	В
65	MOTA	2486	CA	THR	346	45.794	-4.959	65.838	1.00 20.75	В
65	MOTA	2487	CB	THR	346	46.978	-5.579	65.057	1.00 21.69	В
	ATOM	2488		THR	346	47.743	-4.531	64.460	1.00 23.54	В
	MOTA	2489		THR	346	46.486	-6.540	63.964	1.00 20.78	Ð
	ATOM	2490	Ç	THR	346	44.825	-6.070	66.269	1.00 20.06	В
70	MOTA	2491	0	THR	346	43.824	-6.323	65.603	1.00 19.82	В
70	ATOM .	2492	N	LEU	347	45.127	-6.717	67.395	1.00 19.28	В
	MOTA	2493	CA	LEU	347	44.265	-7.771	67.924	1.00 20.23	В
	MOTA	2494	CB	LEU	347	44.967	-8.547	69.080	1.00 20.75	В
	MOTA	2495	CG	LEU	347	46.123	-9.517	68.681	1.00 20.74	В

	MOTA	2496	CD1	LEU	347	46.659 -10	.198 69.923	1.00 18.01	В
	MOTA	2497	CD2	LEU	347	45.630 -10	.563 67.681	1.00 19.87	В
	ATOM	2498	С	LEU	347		.187 68.426		В
	ATOM	2499	ō	LEU	347		.735 68.165		В
5	ATOM	2500	N	SER	348		.074 69.148		В
_									
	MOTA	2501	CA	SER	348		.450 69.645		В
	MOTA	2502	CB	SER	348		.205 70.337		₿
	MOTA	2503	OG	SER	348	42.924 -4	.491 71.458	1.00 23.16	В
	MOTA	2504	С	SER	348	40.848 -5	.161 68.498	1.00 18.64	В
10	ATOM	2505	0	SER	348		.505 68.560		В
	ATOM	2506	N	THR	349		.535 67.447		В
	ATOM	2507	CA	THR	349				
							.195 66.274	1.00 20.04	В
	ATOM	2508	CB	THR	349		.523 65.189		В
1.5	MOTA	2509		THR	349		.195 65.607		В
15	MOTA	2510	CG2	THR	349	40.692 -3	.471 63.848	1.00 20.74	В
	ATOM	2511	С	THR	349	39.873 -5	.402 65.658	1.00 20.94	В
	MOTA	2512	0	THR	349	38.651 -5	.399 65.516		В
	MOTA	2513	N	LEU	350		423 65.280		В
	MOTA	2514	CA	LEU	350		.632 64.682	1.00 25.37	
20									В
20	MOTA	2515	CB	LEU	350		.728 64.483	1.00 24.15	В
	MOTA	2516	CG	LEU	350		.768 63.261		В
	MOTA	2517	CD1	LEU	350	41.548 -7	.931 62.146	1.00 24.69	В.
	MOTA	2518	CD2	LEU	350	43.476 -8	.294 63.652	1.00 25.26	В
	MOTA	2519	С	LEU	350	38.967 -8.	.204 65.570	1.00 25.64	· B
25	ATOM	2520	Ō	LEU	350		651 65.088	1.00 25.79	В
	ATOM	2521	N	GLU	351				
								1.00 26.21	В
	MOTA	2522	CA	GLU	351		.705 67.859	1.00 26.22	В
	ATOM	2523	CB	GLU	351		.729 69.230	1.00 29.30	В
20	MOTA	2524	CG	GLU	351	38.325 -9.	.722 70.181	1.00 35.95	В
30	ATOM	2525	CD	GLU	351	38.148 -11.	.081 69.528	1.00 39.86	В
	ATOM	2526	OE1	GLU	351	39.180 -11.		1.00 39.55	В
	MOTA	2527		GLU	351	36.973 -11.		1.00 40.87	В
	ATOM	2528	c	GLU	351		887 67.927	1.00 24.59	
									B
35	ATOM	2529	0	GLU	351		438 67.987	1.00 24.44	В
23	ATOM .	2530	И	TYR	352		569 67.922	1.00 22.44	В
•	MOTA	2531	CA	TYR	352	36.058 -5.	.627 67.973	1.00 20.05	В
	MOTA	2532	CB	TYR	352	36.638 -4.	176 68.166	1.00 20.78	В
	MOTA	2533	CG	TYR	352		065 68.285	1.00 19.34	В
_	MOTA	2534		TYR	352		539 67.153	1.00 17.81	В
40	ATOM	2535		TYR	352				
70							515 67.258	1.00 19.71	B
	ATOM	2536		TYR	352		535 69.533	1.00 19.30	В
	MOTA	2537		TYR	352		507 69.649	1.00 17.88	В
	ATOM	2538	CZ	TYR	352	33.737 -1.	.003 68.508	1.00 19.50	B
	ATOM	253 9	OH	TYR	352	32.810 0.	017 68.602	1.00 23.10	В
45	ATOM	2540	С	TYR	352		723 66.706	1.00 20.25	В
	ATOM	2541	ō	TYR	352		704 66.776	1.00 20.39	В
	ATOM	2542	N	ALA	353				
							851 65.549	1.00 20.55	В
	ATOM	2543	CA	ALA	353		941 64.289	1.00 23.02	В
50	MOTA	2544	CB	ALA	353		711 63.116	1.00 20.71	В
50	MOTA	2545	С	ALA	353	34.374 -7.	271 64.109	1.00 25.05	B
	MOTA	2546	0	ALA	353	33.259 -7.	299 63.580	1.00 24.67	В
	MOTA	2547	N	HIS	354	34.983 -8.	366 64.553	1.00 26.56	В
	ATOM	2548	CA	HIS	354		682 64.420	1.00 29.08	В
	ATOM	2549	CB	HIS	354	35.332 -10.		1.00 30.47	В
55	MOTA	2550	CG	HIS	354				
55		2551				34.916 -12.		1.00 31.52	В
	MOTA			HIS	354	34.400 -13.		1.00 30.23	В
	ATOM	2552	ND1		354	34.990 -12.		1.00 32.72	В
	MOTA	2553	CEI	HIS	354	34.539 -13.	870 63.222	1.00 32.65	В.
	ATOM	2554	NE2	HIS	354	34.175 -14.	213 64.445	1.00 32.59	B
60	MOTA	2555	С	HIS	354	33.059 -9.		1.00 30.20	В
	ATOM	2556	0	HIS	354	32.075 -10.			
	ATOM	2557	N	ARG				1.00 30.57	В
					355		177 66.390	1.00 31.47	В
	MOTA	2558	CA	ARG	355		166 .67.182	1.00 33.23	В
15	MOTA	2559	CB	ARG	355	32.064 ~8.	504 68.551	1.00 35.96	В
65	MOTA	2560	CG	ARG	355		364 69.516	1.00 40.08	Ð
	MOTA	2561	CD	ARG	355		625 70.797	1.00 43.24	В
	ATOM	2562	NE	ARG	355		198 71.579	1.00 47.90	B
	ATOM	2563	CZ	ARG	355				
							016 72.081	1.00 50.90	В
70	MOTA	2564	NH1		355	31.208 -10.		1.00 50.97	В
<i>1</i> U	ATOM	2565	NH2		355		521 72.806	1.00 50.14	В
	MOTA	2566	С	ARG	355	30.770 -8.	378 66.413	1.00 32.60	В
	ATOM	2567	0	ARG	355		801 66.321	1.00 32.82	В
	ATOM	2568	N	ALA	356		240 65.850	1.00 29.87	В
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	MOTA	2569	CA AL	A 356	30.266	-6.389	65.096	1.00 27.94	В
	MOTA	2570	CB AL						
					31.025	-5.243	64.467	1.00 28.16	В
	MOTA	2571	C AL		29.485	-7.137	64.022	1.00 26.92	В
~	MOTA	2572	O AL		28.356	-6.759	63.698	1.00 24.79	В
5	ATOM	2573	N LY	357	30.074	-8.203	63.486	1.00 25.84	В
	MOTA	2574	CA LY	357	29.416	-8.982	62.438	1.00 27.17	В
	ATOM	2575	CB LY		30.248		62.040	1.00 26.83	В
	ATOM	2576	CG LY		31.690	-9.905	61.724	1.00 28.45	
	ATOM	2577							В
10						-10.857	60.651	1.00 31.56	В
10	ATOM	2578	CE LY		31.933	-12.305	61.008	1.00 31.36	В
	MOTA	2579	NZ LYS	357	32.361	-13.190	59.908	1.00 30.37	В
	ATOM	2580	C LYS	357	28.036	-9.483	62.831	1.00 27.51	В
	MOTA	2581	O LYS	357	27.173	-9.651	61.974	1.00 27.57	В
	MOTA	2582	N ASI		27.829	-9.728	64.121	1.00 28.92	В
15	MOTA	2583	CA ASI			-10.234		1.00 30.60	
	MOTA	2584					64.597		В
			CB ASI			-11.024	65.911	1.00 31.34	В
	ATOM	2585	CG AS			-12.311	65.709	1.00 33.50	В
	MOTA	2586	OD1 AS	358	28.750	-12.292	65.537	1.00 34.98	В
	MOTA	2587	ND2 AS	₹ 358	26.823	-13.439	65.716	1.00 33.36	В
20	ATOM	2588	C ASI	358	25.426	-9.207	64.788	1.00 30.89	В
	MOTA	2589	O ASI		24.367	-9.547	65.302	1.00 32.42	B
	MOTA	2590	N IL		25.642				
						-7.961	64.381	1.00 31.36	В.
	ATOM	2591	CA ILI		24.607	-6.943	64.530	1.00 31.09	В
25	ATOM	2592	CB ILE		25.185	-5.505	64.454	1.00 30.83	В
25	MOTA	2593	CG2 ILE		24.060	-4.493	64.496	1.00 28.14	В
	ATOM	2594	CG1 ILE	359	26.144	-5.246	65.629	1.00 29.88	В
	ATOM	2595	CD1 ILE	359	27.028	-4.031	65.421	1.00 29.12	В
	MOTA	2596	C IL		23.583	-7.110	63.416	1.00 32.70	В
	MOTA	2597	O ILE						
30					23.938	-7.293	62.250	1.00 31.89	B
50	MOTA	2598	N LEU		22.312	-7.045	63.795	1.00 34.93	B
	MOTA	2599	CA LEU		21.195	~7.185	62.869	1.00 37.63	В
	MOTA	2600	CB LEU	7 360	20.056	-7.993	63.544	1.00 39.00	В
	MOTA	2601	CG LET	360	18.581	-7.590	63.189	1.00 41.16	В
	ATOM	2602	CD1 LEU	360	18.283	-7.917	61.728	1.00 42.20	В
35	ATOM	2603	CD2 LEU		17.599	-8.315	64.118	1.00 41.50	В
	ATOM	2604	C LEU		20.672				
	ATOM					-5.814	62.475	1.00 38.26	В
		2605	O LEU		20.356	-5.003	63.343	1.00 38.46	В
	MOTA	2606	n asn		20.580	-5.565	61.171	1.00 39.80	В
40	ATOM	2607	CA ASN	361	20.079	-4.295	60.656	1.00 41.76	В
40	MOTA	2608	CB ASN	361	21.133	-3.606	59.822	1.00 42.66	В
	MOTA	2609	CG ASN	361	22.088	-2.772	60.657	1.00 44.51	В
	ATOM	2610	OD1 ASN		22.791	-3.289	61.528	1.00 45.27	В
	MOTA	2611	ND2 ASN		22.117	-1.467	60.394	1.00 45.23	В
	ATOM	2612	C ASN						
45					18.825	-4:481	59.812	1.00 44.12	В
43	ATOM	2613	O ASN		18.478	-5.604	59.438	1.00 45.59	В
	MOTA	2614	N LYS	362	18.160	-3.366	59.514	1.00 45.40	В
	MOTA	2615	CA LYS		16.931	-3 .332	58.716	1.00 45.80	В
	ATOM	2616	CB LYS	362	17.226	-3.756	57.260	1.00 45.62	В
	MOTA	2617	CG LYS	362	17.222	-2.619	56.240	1.00 45.92	В
50	ATOM	2618	CD LYS		15.832	-2.001	56.093	1.00 45.58	В
	ATOM	2619	CE LYS		15.739				
	ATOM	2620				-1.104	54.862	1.00 43.34	В
					14.456	-0.345	54.818	1.00 42.49	В
	ATOM	- 2621	C LYS		15.823	-4.213	59.292	1.00 47.03	В
F 5	MOTA	2622	O LYS	362	15.150	-4.897	58.492	1.00 48.78	B
55	MOTA	2623	OXT LYS	362	15.624	-4.198	60.526	1.00 47.26	В
	MOTA	2624	MG MG	· 2602	43.330	10.372	60.103	1.00 26.54	
	ATOM	2625	PB ADP		44.452	7.135	60.400	1.00 17.43	ADP
	ATOM	2626	O1B ADP						
				2600	44.951	7.845	61.612	1.00 18.86	ADP
60	ATOM	2627	OZB ADP		44.008	5.637	60.747	1.00 22.98	ADP
OU	ATOM	2628	O3B ADP	2600	43.299	7.848	59.790	1.00 19.76	ADP
	MOTA	2629	PA ADP	2600	45.880	7.608	57.967	1.00 24.97	ADP
	ATOM	2630	Ola ADP	2600	44.906	7.153	56.989	1.00 27.54	ADP
	ATOM	2631	O2A ADP	2600	45.805	9.067	58.061	1.00 29.40	ADP
	ATOM	2632	O3A ADP		45.606	6.967	59.369	1.00 22.28	
65	ATOM	2633	OS* ADP	2600	47.347				ADP
03						7.314	57.518	1.00 28.31	ADP
	ATOM	2634	C5* ADP		48.422	6.620	58.144	1.00 30.71	ADP
	MOTA	2635	C4* ADP	2600	49.601	6.747	57.103	1.00 33.98	ADP
	MOTA	2636	O4* ADP	2600	49.664	5.485	56.457	1.00 33.98	ADP
30	MOTA	2637	C3 ADP	2600	49.383	7.792	55.972	1.00 32.52	ADP
70	MOTA	2638	O3* ADP	2600	50.518	8.657	55.838	1.00 36.94	ADP
	ATOM	2639	C2* ADP	2600	49.106	7.017	54.682		
	MOTA	2640	O2* ADP	2600	49.782			1.00 35.49	ADP
						7.556	53.522	1.00 38.23	ADP
	ATOM	2641	C1 * ADP	2600	49.483	5.577	55.026	1.00 35.20	ADP

	ATOM	2642	N9	ADP	2600	48.437	4.548	54.689	1.00 33.78	ADP
	ATOM	2643	C8	ADP	2600	47.512	4.099	55.567	1.00 34.18	ADP
	ATOM	2644	N7	ADP	2600	46.745	3.202	55.003	1.00 36.36	ADP
5	ATOM	2645	C5	ADP	2600	47.137	3.045	53.768	1.00 36.94	ADP
)	ATOM	2646	C6	ADP	2600	46.721	2.241	52.700	1.00 37.31	ADP
	MOTA	2647	N6	ADP	2600	45.687	1.403	52.874	1.00 37.72	ADP
	MOTA ATOM	2648 2649	N1 C2	ADP ADP	2600	47.381	2.320	51.471	1.00 37.39	ADP
	ATOM	2650	N3	ADP	2600 2600	48.446 48.859	3.171 3.957	51.268	1.00 37.76 1.00 35.88	ADP
10	MOTA	2651	C4	ADP	2600	48.245	3.925	52.311 53.548	1.00 35.51	ADP ADP
	ATOM	2652	Cl	1-7	1	37.929	17.272	54.077	1.00 38.43	1~7
	ATON	2653	C2	1-7	ī	38.932	17.045	53.074	1.00 38.52	1-7
	ATOM	2654	C3	1-7	1	38.735	15.932	52.163	1.00 39.96	1-7
1.5	MOTA	2655	C4	1-7	1	37.528	15.091	52.280	1.00 39.17	1-7
15	ATOM	2656	C5	1-7	1	36.503	15.314	53.268	1.00 37.92	1-7
	MOTA	2657	C6	1-7	1	36.737	16.421	54.166	1.00 39.95	1-7
	MOTA	2658	C11		1	39.781	15.680	51.154	1.00 38.83	1-7
	MOTA	2659	N12		1	40.860	16.465	50.816	1.00 41.41	1-7
20	MOTA MOTA	2660 2661	N13		1	41.632	15.978	49.912	1.00 42.37	1-7
20	ATOM	2662	C14		1 1	41.128 40.183	14.690 14.416	49.355	1.00 40.44	1-7 1-7
	ATOM	2663		1-7	i	41.056	14.226	50.455 47.951	1.00 39.39 1.00 36.95	1-7
	ATOM	2664		1-7	ī	42.809	16.554	49.520	1.00 43.23	1-7
	MOTA	2665		1-7	1	43.706	15.596	48.761	1.00 42.51	1-7
25	MOTA	2666		1-7	1	43.145	17.720	49.767	1.00 44.94	1-7
	MOTA	2667		1-7	1	40.067	14.828	47.075	1.00 35.46	1-7
	MOTA	2668		1-7	1	40.008	14.513	45.661	1.00 35.09	1-7
	MOTA	2669		1-7	1	40.989	13.573	45.157	1.00 34.04	1-7
30	MOTA	2670		1-7	1	41.984	12.977	46.048	1.00 34.13	1-7
50	ATOM ATOM	2671 2672		1-7	1	42.012	13.263	47.467	1.00 34.81	1-7
	ATOM	2673		1-7	1	37.356 42.983	13.776 12.166	51.201	1.00 40.06 1.00 32.08	1-7
	ATOM	2674	0	нон	2	38.525	10.810	45.535 62.766	1.00 32.08	1-7 S
	ATOM	2675	ŏ	нон	3	23.222	11.589	60.100	1.00 22.29	S
35	ATOM	2676	ō	нон	4	41.960	12.208	60.870	1.00 9.69	S
	ATOM	2677	0	нон	5	50.029	-4.994	63.682	1.00 18.21	s
	MOTA	2678	0	нон	8	28.413	21.060	56.800	1.00 20.56	s
	MOTA	2679	0	нон	9	31.397	6.826	80.114	1.00 18.48	S
40	MOTA	2680	0	нон	10	38.337	3.375	65.490	1.00 21.12	s
40	ATOM	2681	0	НОН	13	45.628	22.010	69.140	1.00 9.64	s
	MOTA ATOM	2682	0	нон	14	48.257	14.330	41.733	1.00 18.62	s
	ATOM	2683 2684	0	нон	15 16	41.014	5.558 20.868	71.890 70.581	1.00 28.07	s
	ATOM	2685	ŏ	нон	17	43.663	-1.056	64.226	1.00 22.56 1.00 13.66	s s
45	ATOM	2686	ŏ	нон	18	43.194	8.354	64.240	1.00 19.73	5
	MOTA	2687	ō	нон	20	54.924	6.098	49.933	1.00 32.18	Š
	ATOM	2688	0	нон	22	31.350	4.322	82.668	1.00 37.14	s
	MOTA	2689	0	HOH	27	45.521	-1.603	51.520	1.00 20.22	s
50	MOTA	2690	0	нон	28	53.208	11.559	41.772	1.00 42.11	s
20	ATOM	2691	0	нон	31	27.994	6.504	79.871	1.00 18.94	s
	MOTA MOTA	2692 2693	0	HOH	33	49.291	-7.879	50.486	1.00 35.78	s
	ATOM	2694	0	нон	34	18.468 53.496	12.203	33.372	1.00 19.62	S
	ATOM	2695	ŏ	нон	35 36	45.680	-17.951 3.185	61.642 45.465	1.00 35.98 1.00 19.30	s s
55	ATOM	2696	ō	нон	38	42.176	-0.846	72.113	1.00 14.70	S
	MOTA	2697	0	нон	39	51.304	5.232	60.441	1.00 24.96	S
	MOTA	2698	0	HOH	40	34.806	13.087	70.806	1.00 32.37	s
	MOTA	2699	0	нон	41	19.156	14.294	56.441	1.00 28.63	s
60	MOTA	2700	0	HOH	46	44.126	0.351	55.876	1.00 28.55	S
60	MOTA	2701	0	нон	47	20.432	7.836	62.530	1.00 16.12	s
	MOTA	2702	0	нон	48	31.643	24.934	63.575	1.00 31.65	s
	MOTA	2703	0	HOH	50	45.290	17.359	64.325	1.00 15.86	S
	MOTA	2704	0	нон	53	41.790	5.942	40.546	1.00 28.37	s
65	MOTA MOTA	2705 2706	0	нон	54 55	38.452	4.419	47.214	1.00 14.56	S
	ATOM	2700	0	HOH	55 57	52.009 51.429	4.613	57.096	1.00 35.87	S
	ATOM	2708	0	HOH	5 <i>1</i> 58	22.685	6.864 19.136	39.244	1.00 27.91	s s
	MOTA	2709	ō	нон	61	39.044	12.519	43.047 58.483	1.00 29.36 1.00 28.94	S
	ATOM	2710	ŏ	нон	67	45.314	-7.264	72.406	1.00 28.94	S
70	ATOM	2711	ŏ	нон	69	46.768	-2.040	64.134	1.00 17.23	S
	ATOM	2712	0	HOH	71	45.298	18.821	48.751	1.00 30.98	s
	ATOM	2713	0	нон	79	45.903	11.457	63.308	1.00 21.87	Š
	ATOM	2714	0	нон	83	29.506	-5.557	49.394	1.00 32.50	s

	MOTA	2715	0	нон	86	28.178	4.602	77.098	1.00 29.04	S
	MOTA	2716	0	нон	89	55.210	-16.662	58.167	1.00 35.61	s
	MOTA	2717	0	HOH	91	37.135	0.846	70.878	1.00 20.52	s
_	MOTA	2718	0	нон	93	17.438	19.816	52.756	1.00 35,47	S
5	MOTA	2719	0	нон	94	29.881	3.798	41.417	1.00 42.97	s
	ATOM	2720	0	нон	98	39.190	3.892	49.946	1.00 13.01	s
	MOTA	2721	0	HOH	100	41.671	15.312	56.323	1.00 31.21	s
	MOTA	2722	0	HOH	101	52.876	0.835	68.812	1.00 32.79	S
	MOTA	2723	0	HOH	105	37.722	2.513	73.490	1.00 36.02	s
10	MOTA	2724	0	нон	109	27.450	25.927	61.040	1.00 42.15	S
	MOTA	2725	0	HOH	111	39.804	17.000	76.527	1.00 40.03	S
	MOTA	2726	0	HOH	117	2.532	6.263	36.270	1.00 22.77	S
	MOTA	2727	0	HOH	119	43.756	2.932	43.574	1.00 30.63	S
	MOTA	2728	0	нон	124	41.324	9.248	61.513	1.00 50.60	S
15	MOTA	2729	0	HOH	128	45.349	21.055	46.092	1.00 34.28	S
	MOTA	2730	0	нон	129	47.480	9.402	61.725	1.00 20.53	s
	MOTA	2731	0	нон	130	27.022	14.663	58.188	1.00 21.56	S
•	MOTA	2732	0	HOH	131	38.009	11.637	34.970	1.00 36.04	s
~~	MOTA	2733	0	нон	135	21.462	18.078	39.253	1.00 49.42	s
20	ATOM	2734	0	HOH	136	50.206	-0.381	68.977	1.00 28.73	S
	MOTA	2735	0	нон	142	43.209	19.312	57.176	1.00 32.90	S
	MOTA	2736	0	нон	144	27.420		56.585	1.00 40.61	S
	MOTA	2737	0	HOH	145	56.085	3.298	61.538	1.00 27.46	s
25	MOTA	2738	0	HOH	148	45.044	22.181	54.899	1.00 33.67	S
25	ATOM	2739	0	нон	149	47.168	9.785	68.295	1.00 32.20	S
	MOTA	2740	0	нон	150	35.221	13.107	56.556	1.00 39.71	S
	ATOM	2741	0	нон	156	19.494	13.147	35.697	1.00 37.79	S
	MOTA	2742	0	нон	158	35.348	1.853	79.606	1.00 35.97	S
20	MOTA	2743	0	HOH	160	44.086	-3.335	73.582	1.00 28.68	S
30	MOTA	2744	0	нон	163	22.716	28.692	55.723	1.00 38.12	s
	ATOM END	2745	0	нон	164	29.077	26.837	62.948	1.00 37.04	s
	END									

TABLE 3

	REMARI REMARK					n: 50.0 - 3							
5	REMARK REMARK	rmsd sg= P	bond 2(1)	s= 0. 2(1)2	007673 2(1) a=	rmsd angle 68.9 b= 79	es= 1.23 .4 c= 158		= 90.	beta=	90.	gamma=	90.
	REMARK	FILEN	AME=	Cont	ound 2-	7_3pb.pdb*		•					
	MOTA	1	CB	LYS	17	24.357	-12.099	59.933		58.09		В	
10	MOTA	2	CG	LYS	17		-12.631	59.411		60.84		В	
10	MOTA	3	CD	LYS	17		-12.482	57.896		62.11		В	
	ATOM	4	CE	LYS	17		-13.578	57.123		63.01		В	
	MOTA MOTA	5 6	NZ C	LYS	17 17	25.089	-13.550	57.289		63.35		B	
	ATOM	7	Ö	LYS LYS	17	24.262 25.150	-9.73 7 -9.723	59.096 58.262		54.65 53.83		В	
15	ATOM	8	N	LYS	17		-10.341	61.285		56.25		В	
	MOTA	9	CA	LYS	17		-10.617	60.333		55.82		В	
	MOTA	10	N	ASN	18	23.168	-8.993	58.994		53.57		В	
	ATOM	11	CA	ASN	18	22.956	-8.115	57.857		52.96		В	
. 00	MOTA	· 12	CB	ASN	18	21.634	-7.362	58.018	1.00	55.67		B	
20	MOTA	13	CG	ASN	·18	20.433	-8.197	57.613		58.59		В	
	MOTA	14		asn	18	20.173	-9.261	58.187		59.98		В.	
	MOTA	15		ASN	18	19.688	-7.717	56.621		58.01		В	
	MOTA	16	C	ASN	18	24.093	-7.115	57.635		51.27		В	
25	ATOM	17 18	O N	ASN ILE	18 19	24.391	-6.754	56.495		52.49		B B	
25	MOTA MOTA	19	CA	ILE	19	24.723 25.811	-6.665 -5.698	58.716 58.613		47.11		В	
	MOTA	20	CB	ILE	19	26.192	-5.152	60.004		42.31		В	
	ATOM	21		ILE	19	26.598	-6.295	60.917		43.22		В	
	ATOM	22		ILE	19	27.343	-4.159	59.881		41.90		В	
30	MOTA	23	CD1	ILE	19	27.762	-3.556	61.193	1.00	43.78		В	
	MOTA	24	С	ILE	19	27.054	-6.300	57.958	1.00	38.26		В	
	MOTA	25	.0	ILE	19	27.480	-7.376	58.312		38.23		В	
	ATOM	26	N	GLN	20	27.627	-5.577	56.999		34.90		В	
35	ATOM	27	CA	GLN	20	28.820	-6.021	56.279		30.15		В	
33	MOTA MOTA	28 29	CB	GLN	20 20	28.778	-5.516	54.838		27.85		B B	
	ATOM	30	CG CD	GLN GLN	20	30.034 29.987	-5.802 -5.186	54.038 52.643		26.74 27.60		В	
	MOTA	31		GLN	20	30.137	-3.984	52.484		29.30		В	
	ATOM	32		GLN	20	29.774	-6.017	51.632		26.15		В	
40	ATOM	33	c	GLN	20	30.091	-5.507	56.949		29.28		В	
	MOTA	34	0	GLN	20	30.186	-4.346	57.290		29.19		В	
	MOTA	35	N	VAL	21	31.075	-6.379	57.127	1.00	27.08		В	
	MOTA	36	CA	VAL	21	32.325	-5.975	57.754		24.84		В	
15	MOTA	37	CB	VAL	21	32.448	-6.546	59.180		24.84		В	
45	ATOM	38		VAL	21	33.766	-6.123	59.804		23.30		В	
	ATOM ATOM	39 40	CG2	VAL	21	31.274	-6.078	60.033		24.09		В	
	MOTA	41	0	VAL VAL	21 21	33.524 33.677	-6.439 -7.608	56.938 56.687		24.57 24.54		B B	
	ATOM	42	N	VAL	22	34.370	-5.496	56.531		25.16		В	
50	ATOM	43	CA	VAL	22	35.558	-5.818	55.753		24.51		B	
	MOTA	44	СВ	VAL	22	35.493	-5.171	54.356		25.74		В	
	MOTA	45	CG1	VAL	22	34.274	-5.694	53.602		23.07		В	
	ATOM	46	CG2	VAL	22	35.428	-3.648	54.488	1.00	26.13		В	
55	MOTA	47	С	VAL	22	36.825	-5.350	56.464		24.25		В	
55	MOTA	48	0	VAL	22	36.769	-4.532	57.376		25.41		В	
	ATOM	49	N	VAL	23	37.964	-5.889	56.047		21.62		В	
	ATOM	50	CA	VAL	23	39.249	-5.541	56.640		20.21		В	
	MOTA MOTA	51 52	CB	VAL	23 23	39. 875 41.246	-6.749 -6.386	57.398 57.920		19.81 17.77		B B	
60	MOTA	53		VAL	23	38.980	-7.164	58.552		19.57		В	
00	ATOM	54	C	VAL	23	40.224	-5.069	55.565		20.21		В	
	MOTA	55	ŏ	VAL	23	40.231	-5.587	54.453		18.34		В	
	ATOM	56	N	ARG	24	41.026	-4.063	55.908		20.97		. B	
	ATOM	57	CA	ARG	24	42.012	-3.508	54.987		23.76		B	
65	MOTA	58	CB	ARG	24	41.493	-2.221	54.341	1.00	19.71		В	
	MOTA	59	CG	ARG	24	42.364	-1.729	53.201		19.19		В	
	ATOM	60	CD	ARG	24	42.064	-0.294	52.784		17.94		В	
	ATOM	61	NE	ARG	24	42.664	0.010	51.487		16.57		В	
70	MOTA	62	CZ	ARG	24	42.479	1.134	50.801		18.90		В	
70	ATOM	63 64		ARG	24	41.704	2.100	51.281		16.81		B	
	MOTA	04	MUZ	ARG	24	43.057	1.275	49.615	1.00	16.05		D	

	MOTA	65	С	ARG	24	43.304	-3.210	55.736	1.00 27.05	В
	MOTA	66	0	ARG	24	43.313	-2.442	56.712	1.00 27.85	В
	ATOM	67	N	CYS	25					
						44.392	-3.820	55.274	1.00 29.51	В
_	MOTA	68	CA	CYS	25	45.699	-3.637	55.890	1.00 32.32	В
5	ATOM	69	CB	CYS	25	46.410	-4.991	56.027	1.00 30.86	В
	MOTA	70	SG	CYS	25	48.111	-4.890	56.627	1.00 32.54	В
	MOTA	71	C	CYS	25	46.545	-2.696	55.045	1.00 33.84	B
	MOTA	72	0	CYS	25	46.587	-2.820	53.831	1.00 35.92	В
• •	ATOM	73	N	ARG	26	47.218	-1.754	55.694	1.00 34.94	В
10	MOTA	74	CA	ARG	26	48.053	-0.807	54.967	1.00 37.11	В
	ATOM	75	CB	ARG	26	48.130	0.526	55.723	1.00 37.77	В
	MOTA	76	CG	ARG	26					
						48.388	0.384	57.222	1.00 37.85	В
	MOTA	77	CD	ARG	26	49.107	1.591	57.802	1.00 36.08	В
. ~	ATOM	78	NE	ARG	26	50.554	1.433	57.704	1.00 35.38	В
15	MOTA	79	CZ	ARG	26	51.379	1.390	58.747	1.00 35.56	В
	ATOM	80	NH1		26	50.910	1.502	59.982	1.00 32.33	В
	ATOM	81		ARG	26	52.677				
							1.209	58.551	1.00 37.10	В
	MOTA	82	С	ARG	26	49.463	-1.341	54.751	1.00 38.55	В
	ATOM	83	0	ARG	26	49.917	-2.224	55.460	1.00 38.07	В
20	MOTA	84	N	PRO	27	50.170	-0.806	53.752	1.00 40.05	В
	ATOM	85	CD	PRO	27	49.674	0.092	52.693	1.00 41.26	В
	MOTA	86	CA	PRO	27					
						51.536	-1.244	53.467	1.00 42.07	В
	ATOM	87	CB	PRO	27	51.734	-0.805	52.021	1.00 42.46	В
~-	MOTA	88	CG	PRO	27	50.945	0.468	51.961	1.00 41.54	В
25	MOTA	89	С	PRO	27	52.508	~0.555	54.418	1.00 43.29	В
	ATOM	90	o	PRO	27	52.115	0.329	55.170	1.00 43.49	В
	MOTA	91	N	PHE	28	53.773				
							-0.968	54.380	1.00 45.76	В
	MOTA	92	CA	PHE	28	54.807	-0.381	55.233	1.00 47.49	В
~~	MOTA	93	CB	PHE	28	56.045	-1.290	55.308	1.00 46.30	В
30	MOTA	94	CG	PHE	28	55.770	-2.659	55.861	1.00 45.96	В
	ATOM	95		PHE	28	55.424	-3.709	55.015	1.00 45.49	В
	ATOM	96		PHE	28	55.849				
							-2.899	57.230	1.00 45.19	В
	MOTA	97		PHE	28	55.162	-4.976	55.526	1.00 44.86	₽
25	MOTA	98	CE2	PHE	28	55.588	-4.165	57.751	1.00 44.92	В
35	MOTA	99	CZ	PHE	28	55.244	-5.204	56.897	1.00 43.96	В
•	MOTA	100	С	PHE	28	55.240	0.974	54.686	1.00 49.68	В
	MOTA	101	ŏ	PHE	28					
						55.458	1.127	53.484	1.00 50.76	В
	ATOM	102	N	ASN	29	55.369	1.955	55.572	1.00 51.78	В
**	ATOM	103	CA	ASN	29	55.791	3.289	55.164	1.00 53.98	В
40	ATOM	104	CB	ASN	29	55.477	4.303	56.268	1.00 52.37	В
	ATOM	105	CG	ASN	29	55.889	3.818	57.647	1.00 51.95	В
	MOTA	106		ASN	29	57.068				
							3.614	57.918	1.00 51.68	В
	MOTA	107		ASN	29	54.909	3.633	58.526	1.00 50.23	В
40	MOTA	108	С	ASN	29	57.285	3.275	54.841	1.00 56.89	В
45	ATOM	109	0	ASN	29	57.973	2.293	55.111	1.00 57.68	В
	ATOM	110	N	LEU	30	57.779	4.361	54.257	1.00 59.05	В
	ATOM	111	CA	LEU	30	59.185	4.452	53.882	1.00 60.93	В
	MOTA	112	CB	LEU	30	59.466	5.837	53.293	1.00 60.81	B
50	ATOM	113	CC	LEU	30	60.555	5.909	52.218	1.00 61.25	В
50	ATOM	114	CD1	LEU	30	60.401	7.199	51.429	1.00 61.39	₿
	MOTA	115	CD2	LEU	30	61.935	5.810	52.856	1.00 61.13	В
	ATOM	116	C	LEU	30	60.136	4.167	55.047	1.00 62.80	В
	ATOM	117	ō	LEU	30 ·	61.206		54.852		
							3.611		1.00 63.36	В
55	ATOM	118	N	ALA	31	59.736	4.545	56.257	1.00 64.56	В
55	MOTA	119	CA	ALA	31	60.565	4.326	57.440	1.00 66.24	В
	ATOM	120	CB	ALA	31	59.999	5.104	58.617	1.00 64.93	В
	MOTA	121	С	ALA	31	60.671	2.845	57,798	1.00 68.38	В
	ATOM	122	ō	ALA	31	61.757	2.345			
								58.088	1.00 69.26	В
40	MOTA	123	N	GLU	32	59.537	2.153	57.781	1.00 69.84	В
60	MOTA	124	CA	GLU	32	59.492	0.734	58.107	1.00 71.88	В
	MOTA	125	CB	GLU	32	58.038	0.275	58.225	1.00 70.67	В
	MOTA	126	CG	GLU	32	57.338	0.752	59.487	1.00 67.99	В
	ATOM	127	CD	GLU	32		0.607			
						55.831		59.412	1.00 65.98	В
65	MOTA	128		GLU	32	55.174	0.723	60.468	1.00 65.36	В
65	MOTA	129	OE2	GLU	32	55.302	0.383	58.301	1.00 62.48	В
	ATOM	130	С	GLU	32	60.232	-0.143	57.097	1.00 74.40	В
	ATOM	131	ō	GLU	32	61.090	-0.930	57.472	1.00 74.92	В
		132	N							
	MOTA			ARG	33	59.897	-0.008	55.816	1.00 76.35	B
70	MOTA	133	CA	ARG	33	60.550	~0.803	54.779	1.00 78.32	В
70	MOTA	134	CB	ARG	33	59.936	-0.502	53.407	1.00 79.77	В
	ATOM	135	CG	ARG	33	59.972	0.964	53.010	1.00 83.18	В
	ATOM	136	CD	ARG	33	59.329	1.183	51.645	1.00 85.46	В
	ATOM	137	NE							
	AIOM	131	NE.	ARG	33	60.032	0.459	50.589	1.00 87.40	В

	MOTA	138	CZ	ARG	33	61.269	0.737	50.186	1.00 88.75	В
	MOTA	139	NHl	AKG	33	61.948	1.729	50.747	1.00 89.79	В
	MOTA	140	NH2	ARG	33	61.828	0.019	49.221	1.00 89.07	В
-	NOTA	141	С	ARG	33	62.053	-0.536	54.754	1.00 78.80	В
5	ATOM	142	0	ARG	33	62.832	-1.379	54.318	1.00 78.36	B
								55.226		
	MOTA	143	N	LYS	34	62.448	0.644		1.00 79.39	В
	ATOM ·	144	CA	LYS	34	63.853	1.029	55.284	1.00 80.19	В
	MOTA	145	CB	LYS	34	63.984	2.543	55.504	1.00 81.11	В
	MOTA	146	CG	LYS	34	64.392	3.347	54.267	1.00 82.59	В
10										
10	ATOM	147	CD	LYS	34	65.910	3.501	54.147	1.00 83.41	В
	MOTA	148	. CE	LYS	34	66.604	2,186	53.810	1.00 84.19	В
	MOTA	149	NZ	LYS	34	68.089	2.305	53.845	1.00 84.38	В
	MOTA	150	С	LYS	34	64.539	0.285	56.423	1.00 80.45	B
			ō	LYS	34		0.159	56.448	1.00 81.20	В
1 5	MOTA	151	v			65.757				
15	MOTA	152	N	ALA	35	63.740	-0.209	57.365	1.00 80.19	В
	MOTA	153	CA	ALA	35	64.264	-0.946	58.509	1.00 79.99	В
	MOTA	154	CB	ALA	35	63.654	-0.405	59.800	1.00 79.19	В
	MOTA	155	c ·	ALA	35	63.966	-2.441	58.372	1.00 79.54	В
	MOTA	156	0	ALA	35	64.029	-3.181	59.347	1.00 79.52	В
20	MOTA	157	N	SER	36	63.650	-2.870	57.150	1.00 79.23	В
	MOTA	158	CA	SER	36	63.324	-4.269	56.866	1.00 78.90	В
	ATOM	159	CB	SER	`36	64.581	-5.140	56.934	1.00 79.55	В
	ATOM	160	OG	SER	36	65.497	-4.786	55.913	1.00 80.94	В
	MOTA	161	С	SER	36	62.291	-4.773	57.863	1.00 77.94	- B
25										
23	MOTA	162	0	SER	36	62.621	-5.460	58.826	1.00 78.06	В
	MOTA	163	N	ALA	37	61.033	-4.422	57.620	1.00 76.14	В
	MOTA	164	CA	ALA	37	59.952	-4.822	58.505	1.00 74.02	В
	ATOM	165	CB	ALA	37	58.862	-3.763	58.496	1.00 74.76	В
	MOTA	166			37	59.370	-6.177	58.128	1 00 72 22	В
20			С	ALA					1.00 72.27	
30	ATOM	167	0	ALA	37	59.282	~6.526	56.956	1.00 71.83	В
						58.975				В
	MOTA	168	Ŋ	HIS	38		-6.928	59.151	1.00 70.33	
	MOTA	169	CA	HIS	38	58.388	-8.249	58.981	1.00 67.10	В
	MOTA	170	CB	HIS	38	59.039	-9.236	59.961	1.00 69.95	В
	MOTA	171	CG	HIS	38	59.177	-8.706	61.358	1.00 72.03	В
35	MOTA	. 172	CD2	STH	38	58.589	-9.085	62.518	1.00 72.68	В
.00										
	MOTA	173	NDI	HIS	38	60.004	-7.648	61.676	1.00 72.05	В
	MOTA	174	CE1	2TH	38	59.919	-7.399	62.971	1.00 72.38	В
	ATOM	175	NE2	HIZ	38	59.067	-8.256	63.505	1.00 73.14	В
	ATOM	176	С	HIS	38	56.877	-8.187	59.220	1.00 63.55	В
40										
40	MOTA	177	0	HIS	38	56.426	-7.917	60.335	1.00 63.33	В
	ATOM	178	N	SER	39	56.100	-8.432	58.168	1.00 58.67	B
	MOTA	179	CA	SER	39	54.643	-8.399	58.266	1.00 54.45	В
	MOTA	180	CB	SER	39	54.005	-8.478	56.879	1.00 53.84	В
40	MOTA	181	OG	SER	39	52.595	-8.614	56.976	1.00 49.31	В
45	ATOM	182	С	SER	39	54.081	-9.519	59.122	1.00 52.25	В
	ATOM	183	ō		39			58.910		В
				SER			-10.686		1.00 51.84	
	ATOM	184	N	ILE	40	53.251	-9.149	60.089	1.00 49.22	В
	MOTA	185	CA	ILE	40		-10.122	60.967	1.00 47.52	В
	MOTA	186	CB	ILE	40	52.679	-9.674	62.444	1.00 45.91	В
50	MOTA	187	CG2	TIF	40	54.115	-9.499	62.881	1.00 44.82	В
	MOTA	188	CG1	ILE	40	51.915	-8.361	62.622	1.00 45.54	В
	MOTA	189	CD1	ILE	40	51.580	-8.050	64.066	1.00 46.62	В
	MOTA	190	С	ILE	40		-10.316	60.557	1.00 47.28	В
	MOTA	191	0	ILE	40	50.421	-10.994	61.234	1.00 46.90	В
55	ATOM	192	N	VAL	41	50.798	-9.718	59.433		В
55									1.00 47.41	
	MOTA	193	CA	VAL	41	49.430	-9.824	58.939	1.00 48.95	В
	MOTA	194	СВ	VAL	41	48.713	-8.450	58.983	1.00 49.16	В
	ATOM	195	CG1	VAL	41	47.290	-8.585	58.467	1.00 49.01	B.
	ATOM	196	CG2		41	48.713	-7.903	60.402	1.00 49.06	В
60										
60	ATOM	197	С	VAL	41	49.395	-10.347	57.509	1.00 49.67	В
	MOTA	198	0		41	50.004	-9.777	56.620	1.00 49.95	В
				VAL						
	MOTA	199	N	GLU	42	48.685	-11.449	57.301	1.00 50.48	В
	MOTA	200	CA	GLU	42		-12.024	55.969	1.00 51.59	В
	ATOM	201	CB	GLU	42	49.176	-13.434	55.935	1.00 52.66	В
65	ATOM	202		GLU	42		-13.510	56.447	1.00 56.16	В
0.5										
	MOTA	203	CD	GLU	42	51.164	-14.931	56.476	1.00 58.24	В
	MOTA	204	OE1		42		-15.854	56.899	1.00 57.80	В
	ATOM	205	OE2	GLU	42		-15.119	56.081	1.00 58.28	В
	ATOM	206		GLU	42	47.102	-12.072	55.599	1.00 50.83	В
70										
70	MOTA	207	0	GLU	42	46.283	-12.604	56.343	1.00 51.55	В
	ATOM	208	N	CYS	43	46.768	-11.493	54.453	1.00 49.80	В
	MOTA	209		CYS	43		-11.473	53.995	1.00 49.65	В
	ATOM	210		CYS	43 .	45.037	-10.087	53.433	1.00 49.93	Э
		-10				-5.057	20.007		47.73	~

	ATOM	211	SG	CYS	43	45.019 -8.745	54.661	1.00 48.78	В
	ATOM	212	c	CYS	43	45.140 -12.535	52.931	1.00 48.94	В
	MOTA	213	ŏ	CYS	43	46.010 -12.833	52.123	1.00 48.97	
									В
5	MOTA	214	N	ASP	44	43.939 -13.105	52.954	1.00 49.14	В
J	MOTA	215	CA	ASP	44	43.534 -14.121	51.992	1.00 48.86	В
	MOTA	216	CB	ASP	44	43.463 -15.494	52.660	1.00 50.97	В
	ATOM	217	CG	ASP	44	43.589 -16.635	51.666	1.00 52.32	В
	ATOM	218	OD3	ASP	44	43.126 -16.483	50.510	1.00 52.22	В
	ATOM	219		ASP	44	44.147 - 17.689	52.048	1.00 52.81	В
10									
10	ATOM	220	С	ASP	44	42.150 -13.749	51.456	1.00 48.60	В
	MOTA	221	0	ASP	44	41.127 -14.147	52.012	1.00 46.42	В
	MOTA	222	N	PRO	45	42.108 -12.969	50.364	1.00 48.35	В
	MOTA	223	CD	PRO	45	43.252 -12.517	49.557	1.00 48.19	В
	ATOM	224	CA	PRO	45	40.847 -12.540	49.755	1.00 48.75	В
15	ATOM	225	CB	PRO	45				
							48.584	1.00 49.00	В
	MOTA	226	CG	PRO	45	42.617 -12.306	48.211	1.00 49.04	В
	ATOM	227	С	PRO	45	39.957 -13.688	49.312	1.00 50.08	В
	MOTA	228	0	PRO	45	38.750 -13.661	49.535	1.00 50.55	В
	MOTA	229	N	VAL	46	40.561 -14.693	48.683	1.00 50.66	В
20	ATOM	230	CA	VAL	46	39.818 -15.851	48.213	1.00 50.49	В
	ATOM	231	СВ	VAL	46	40.745 -16.853	47.500	1.00 50.30	В
	ATOM.	232							
				VAL	46	39.957 -18.079	47.077	1.00 49.67	В
	ATOM	233	CG2		46	41.393 -16.192	46.293	1.00 49.30	В
0.5	MOTA	234	С	VAL	46	39.145 -16.545	49.389	1.00 50.88	. В
25	MOTA	235	0	VAL	46	37.965 -16.870	49.33B	1.00 52.16	• в
	ATOM	236	N	ARG	47	39.906 -16.761	50.454	1.00 49.91	В
	ATOM	237	CA	ARG	47	39.369 -17.417	51.635	1.00 49.25	В
	ATOM	238	CB	ARG	47	40.499 -18.074			
							52.431	1.00 53.01	В
30	MOTA	239	CG	ARG	47	40.025 -19.009	53.535	1.00 58.79	В
20	MOTA	240	CD	ARG	47	39.711 -20.404	52.993	1.00 62.76	В
	MOTA	241	NE	ARG	47	40.925 -21.094	52.566	1.00 65.61	В
	MOTA	242	CZ	ARG	47	41.887 -21.489	53.395	1.00 67.31	В
	MOTA	243	NH1	ARG	47	41.770 -21.265	54.699	1.00 67.77	В
	ATOM	244		ARG	47	42.970 -22.093	52.922	1.00 67.97	В
35	ATOM	245		ARG	47	38.649 -16.396			
55			C				52.518	1.00 46.27	В
	ATOM	246	0	ARG	47	37.980 -16.767	53.479	1.00 45.17	В
	ATOM	247	N	LYS	48	38.789 -15.116	52.167	1.00 43.30	В
	ATOM	248	CA	LYS	48	38.191 -14.003	52.911	1.00 40.30	В
	MOTA	249	CB	LYS	48	36.660 -14.063	52.861	1.00 40.48	В
40	ATOM	250	CG	LYS	48	36.074 -13.999	51.466	1.00 42.10	В
	ATOM	251	CD	LYS	48	34.566 -14.224	51.491	1.00 46.49	В
	ATOM	252	CE	LYS	48	34.011 -14.463			
							50.088	1.00 48.94	В
	MOTA	253	NZ	LYS	48	34.342 -13.358	49.137	1.00 51.33	В
15	ATOM	254	С	LYS	48	38.649 -14.040	54.364	1.00 38.40	В
45	ATOM	255	0	LYS	48	37.879 -13.780	55.271	1.00 37.06	В
	MOTA	256	N	GLU	49	39.918 -14.374	54.573	1.00 38.43	В
	ATOM	257	CA	GLU	49	40.472 -14.451	55.918	1.00 38.68	В
	ATOM	258	CB	GLU	49	40.965 -15.867	56.237	1.00 42.04	В
	ATOM	259	CG	GLU	49	39.896 -16.940	56.342		
50								1.00 47.74	В
50	MOTA	260	CD	CLU	49	40.478 -18.320	56.671	1.00 49.86	В
	MOTA	261		CLU	. 49	39.706 -19.305	56.666	1.00 50.42	В
	MOTA	262	OE2	CLU	49	41.701 -18.419	56.930	1.00 49.85	В
	ATOM	263	C	GLU	49	41.643 -13.506	56.111	1.00 37.41	В
	ATOM	264	0	GLU	49	42.273 -13.066	55.158	1.00 34.84	В
55	MOTA	265	N	VAL	50	41.925 -13.220	57.374	1.00 36.48	В
	ATOM	266	CA	VAL	50	43.035 -12.366	57.751		
								1.00 37.37	В
	MOTA	267	CB	VAL	50	42.539 -10.930	58.146	1.00 37.30	В
	MOTA	268	CG1		50	41.332 -11.008	59.061	1.00 38.02	В
	MOTA	269	CG2	VAL	50	43.655 -10.153	58.813	1.00 36.20	В
60	MOTA	270	С	VAL	50	43.709 -13.074	58.921	1.00 36.84	В
	MOTA	271	0	VAL	50	43.078 -13.354	59.926	1.00 37.07	В
	ATOM	272	N	SER	51	44.988 -13.399	58.772		В
								1.00 37.03	
	MOTA	273	CA	SER	51	45.702 -14.095	59.835	1.00 37.03	В
65	ATOM	274	CB	SER	51	46.315 -15.390	59.294	1.00 37.38	В
65	ATOM	275	OG	SER	51	46.507 -16.327	60.339	1.00 38.42	В
	MOTA	276	С	SER	51	46.791 -13.217	60.436	1.00 37.30	В
	ATOM	277	0	SER	51	47.538 -12.567	59.712	1.00 37.32	В
	ATOM	278	N	VAL	52	46.870 -13.207	61.764	1.00 37.43	В
	ATOM	279	CA	VAL	52				
70						47.861 -12.398	62.476	1.00 40.09	В
70	MOTA	280	CB	VAL	52	47.170 -11.380	63.433	1.00 38.82	В
	ATOM	281	CG1		52	48.210 -10.529	64.140	1.00 38.44	В
	MOTA	282	CG2	VAL	52	46.207 -10.507	62.664	1.00 39.75	В
	MOTA	283	С	VAL	52	48.814 -13.254	63.307	1.00 41.41	В
							/		_

	MOTA	284	0	VAL	52	48.383	-14.120	64.059	1.00 42.26	В
	MOTA	285	N	ARG	53		-13.001	63.170	1.00 42.93	В
	ATOM	286	CA	ARG	53		-13.746	63.922	1.00 44.63	В
				ARG					1.00 44.03	
5	ATOM	287	CB		53		-13.782	63.156		В
5	MOTA	288	œ	ARG	53		-14.258	63.976	1.00 45.18	В
	MOTA	289	CD	ARG	53	54.721	~14.772	63.069	1.00 47.32	В
	MOTA	290	NE	ARG	53	55.045	-13.815	62.016	1.00 48.93	В
	MOTA	291	CZ	ARG	53	55.538	-14.154	60.831	1.00 48.81	В
	MOTA	292		ARG	53		-15.430	60.548	1.00 49.29	В
10	ATOM	293		ARG	53		-13.221	59.928	1.00 50.89	В
10										
	MOTA	294	С	ARG	53		-13.130	65.298	1.00 46.43	В
	MOTA	295	0	ARG	53		-12.030	65.420	1.00 47.02	В
	MOTA	296	N	THR	54	50.915	-13.855	66.331	1.00 48.25	В
	MOTA	297	CA	THR	54	51.052	-13.401	67.711	1.00 50.92	В
15	MOTA	298	CB	THR	54	49.768	-13.683	68.512	1.00 50.31	В
-	ATOM	299		THR	54		-15.098	68.631	1.00 50.23	В
	ATOM	300		THR	54		-13.078	67.810	1.00 50.24	В
										В
	MOTA	301	С	THR	54		-14.097	68.412	1.00 53.34	
20	MOTA	302	0	THR	54		-13.769	69.538	1.00 53.13	В
20	MOTA	303	N	GLY	55		-15.059	67.726	1.00 57.17	В
	MOTA	304	CA	GLY	55	53.917	-15.805	68.303	1.00 61.42	В
	MOTA	305	С	GLY	[.] 55	55.300	-15.366	67.868	1.00 64.33	В
	MOTA	306	0	GLY	55		-14.175	67.715	1.00 65.05	B
	MOTA	. 307	N	GLY	56		-16.346	67.672	1.00 66.22	В
25		308	CA	GLY	56		-16.061	67.272	1.00 68.09	В
23	ATOM									
	MOTA	309	C	GLY	56		-15.914	65.777	1.00 69.96	В
	MOTA	310	0	GLY	56		-15.305	65.084	1.00 70.41	В
	MOTA	311	N	LEU	57		-16.484	65.288	1.00 71.01	8
	MOTA	312	CA	LEU	57	59.220	-16.421	63.873	1.00 70.64	В
30	MOTA	313	CB	LEU	57	60.702	-16.771	63.704	1.00 71.42	B
	· ATOM	314	CG	LEU	57	61.326	-17.671	64.778	1.00 71.92	В
	MOTA	315		LEU	57		-19.034	64.777	1.00 72.30	В
	MOTA	316	CD2		57	62.819	-17.813	64.522	1.00 72.27	В
										В
.35	ATOM	317	C	LEU	57		-17.311	62.973	1.00 70.34	
دد.		. 318	0	LEU	57	57.535	-18.083	63.450	1.00 69.85	В
	MOTA	319	N	ALA	58		-17.189	61.667	1.00 69.38	В
	MOTA	320	CA	ALA	58	57.852	-17.959	60.669	1.00 68.14	В
	ATOM	321	CB	ALA	58	58.169	-17.430	59.268	1.00 68.25	В
	MOTA	322	С	ALA	58	58.129	-19.462	60.742	1.00 66.52	В
40	ATOM	323	0	ALA	58		-20.268	60.433	1.00 66.64	В
	ATOM	324	N	ASP	59		-19.825	61.150	1.00 64.49	В
				ASP	59	59.743	-21.226	61.270	1.00 62.67	B
	MOTA	325	CA							
	MOTA	326	CB	ASP	59		-21.310	61.798	1.00 62.19	В
4.5	MOTA	327	CG	ASP	59		-22.724	62.197	1.00 61.33	В
45	MOTA	328	OD1	ASP	59	61.727	-23.594	61.307	1.00 59.84	В
	MOTA	329	OD2	ASP	59	61.772	-22.963	63.410	1.00 60.73	В
	MOTA	330	C.	ASP	59	58.801	-21.994	62.201	1.00 61.33	В
	ATOM	331	0	ASP	59		-23.182	62.005	1.00 60.81	В
	ATOM	332	N	LYS	60		-21.302	63.211	1.00 59.03	В
50					60			64.179	1.00 57.28	В
50	MOTA	333	CA	LYS			-21.897			
	MOTA	334	CB	LYS	60		-22.816	65.134	1.00 57.38	B
	MOTA	335	CG	LYS	60		-23.524	66.164	1.00 57.92	B
	MOTA	336	CD	LYS	60	58.117	-24.299	67.172	1.00 58.61	В
	MOTA	337	CE	LYS	60	57.247	-24.930	68.245	1.00 58.86	В
55	ATOM	338	NZ	LYS	60	58.064	-25.535	69.333	1.00 59.92	В
	ATOM	339	C	LYS	60		-20.771	64.968	1.00 55.75	В
	MOTA	340		LYS	60		-19.942	65.574	1.00 55.85	В
										В.
	MOTA	341	N	SER	61		-20.735	64.953	1.00 52.88	
(0	MOTA	342	CA	SER	61		-19.692	65.666	1.00 50.87	В
60	MOTA	343	CB	SER	61	54.863	-18.343	64.967	1.00 50.80	В
	MOTA	344	0G	SER	61	54.294	-18.346	63.667	1.00 48.16	В
	MOTA	345	С	SER	61	53.158	-19.957	65.796	1.00 50.20	В
	ATOM	346	ō	SER	61		-20.909	65.245	1.00 49.59	В
	ATOM	347	N	SER	62		-19.086	66.547	1.00 49.11	В
65										
U	MOTA	348	CA	SER	62		-19.170	66.752	1.00 48.21	В
	MOTA	349	CB	SER	62		-19.101	68.248	1.00 48.08	В
	MOTA	350	OG	SER	62		-17.993	68.858	1.00 48.30	В
	MOTA	351	С	SER	62	50.421	-17.990	66.010	1.00 48.13	В
	ATOM	352	0	SER	62		-17.016	65.703	1.00 47.13	В
70	MOTA	353	N	ARG	63		-18.085	65.712	1.00 47.13	В
	ATOM	354	CA	ARG	63		-17.015	64.998	1.00 45.05	В
										В
	ATOM	355	CB.	ARG	63		-17.231	63.481	1.00 44.51	
	ATOM	356	CG	ARG	63	49.960	-17.194	62.925	1.00 44.98	В

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	MOTA	357	CD	ARG	63	49.976 -17.466	61.428	1.00 46.63	В
	MOTA	358	NE	ARG	63	49.443 -16.349	60.645	1.00 48.69	В
	MOTA	359	CZ	ARG	63	50.148 -15.285	60.263	1.00 48.66	В
	ATOM	360	NH1	ARG	63	51.429 -15.178	60.587	1.00 49.48	В
5	ATOM	361	NH2	ARG	63	49.574 -14.329	59.545	1.00 48.53	В
-	ATOM	362	C	ARG	63	46.975 -16.918	65.401	1.00 43.84	В
				ARG					
	MOTA	363	0		63	46.477 -17.726	66.176	1.00 44.06	В
	MOTA	364	N	LYS	64	46.305 -15.902	64.868	1.00 42.24	В
	ATOM	365	CA	LYS	64	44.89215.652	65.124	1.00 40.40	В
10	MOTA	366	CB	LYS	64	44.723 -14.434	66.032	1.00 41.92	В
	ATOM	367	CG	LYS	64	45.181 -14.635	67.470	1.00 43.37	В
	ATOM	368	CD	LYS	64	44.088 -15.261	68.317	1.00 43.81	В
	ATOM	369	CE	LYS	64	44.446 -15.213	69.794	1.00 45.77	В
1.5	MOTA	370	NZ	LYS	64	43.374 -15.792	70.658	1.00 46.88	В
15	MOTA	371	С	LYS	64	44.257 -15.369	63.771	1.00 39.22	B
	MOTA	372	0	LYS	64	44.631 -14.405	63.102	1.00 39.99	B
	ATOM	373	N	THR	65	43.312 -16.210	63.361	1.00 36.46	В
	MOTA	374	CA	THR	65	42.656 -16.031	62.074	1.00 34.76	В
20	MOTA	375	CB	THR	65	42.745 -17.323	61.212	1.00 35.41	В
20	MOTA	376	OG1	THR	65	44.118 -17.692	61.041	1.00 32.86	В
	ATOM	377	CG2	THR	65	42.130 -17.090	59.826	1.00 36.73	В
	MOTA	378	С	THR	65	41.194 -15.638	62.238	1.00 34.16	В
	MOTA	379	0	THR	65	40.477 -16.200	63.070	1.00 35.43	В
	ATOM	380	N	TYR	66	40.764 -14.660	61.448	1.00 30.66	В
25									
23	MOTA	381	CA	TYR	66	39.391 -14.181	61.488	1.00 28.38	В
	ATOM	382	CB	TYR	66	39.337 -12.765	62.072	1.00 25.32	₿
	MOTA	383	CG	TYR	66	39.886 -12.652	63.473	1.00 22.38	В
	MOTA	384	CD1	TYR	66	41.255 -12.566	63.710	1.00 20.36	В
	HOTA	385	CE1	TYR	66	41.753 -12.475	65.011	1.00 19.50	В
30	ATOM	386	CD2		66	39.027 -12.647	64.569	1.00 22.45	В
	ATOM	387		TYR	66	39.506 -12.559			В
							65.868	1.00 19.18	
	MOTA	388	CZ	TYR	66	40.865 -12.470	66.086	1.00 21.06	В
	MOTA	389	OH	TYR	66	41.317 -12.358	67.391	1.00 25.17	В
~ -	MOTA	390	С	TYR	66	38.815 -14.171	60.076	1.00 29.18	В
35	MOTA	391	0	TYR	66	39.537 -13.953	59.108	1.00 29.59	В
	ATOM	392	N	THR	67	37.514 -14.418	59.963	1.00 30.96	В
	MOTA	393	CA	THR	67	36.854 -14.420	58.662	1.00 31.82	В
	ATOM								
		394	CB	THR	67	36.083 -15.742	58.418	1.00 31.49	В
àΩ	MOTA	395		THR	67	36.983 -16.849	58.543	1.00 35.18	В
40	MOTA	396	CG2	THR	67	35. 482 -15 .759	57.016	1.00 30.30	₿
	MOTA	397	С	THR	67	35.873 -13.252	58.565	1.00 31.85	В
	MOTA	398	0	THR	67	35.100 -12.996	59.504	1.00 32.04	В
	MOTA	399	N	PHE	68	35.923 -12.536	57.442	1.00 29.70	В
	ATOM	400	CA	PHE	68	35.029 -11.400	57.203	1.00 31.18	В
45									
73	MOTA	401	СВ	PHE	68	35.785 - 10.063	57.305	1.00 29.26	В
	MOTA	402	CG	PHE	68.	36.374 -9.797	58.658	1.00 27.25	В
	MOTA	403	CD1	PHE	68	37.617 -10.309	59.001	1.00 28.36	В
	MOTA	404	CD2	PHE	68	35.666 -9.071	59.611	1.00 28.98	В
	ATOM	405	CE1	PHE	68	38.147 -10.110	60.277	1.00 27.66	В
50	ATOM	406	CE2		68	36.188 -8.867	60.894	1.00 27.30	В
	ATOM	407	CZ	PHE	68	37.430 -9.388	61.225	1.00 26.68	В
	ATOM	408	c	PHE	68	34.418 -11.527	55.815	1.00 30.88	В
	MOTA	409	0	PHE	68	34.814 -12.385	55.032	1.00 32.33	В
	MOTA	410	N	ASP	69	33.452 -10.670	55.514	1.00 30.45	В
55	ATOM	411	CA	ASP	69	32,796 -10.702	54.212	1.00 31.77	В
	MOTA	412		ASP	69	31.636 -9.698	54.185	1.00 33.60	В
	ATOM	413		ASP	69	30.590 -9.988	55.258	1.00 36.34	В
	ATOM	414	OD1		69	30.514 -9.221	56.254	1.00 35.89	В
(0	MOTA	415	OD2	ASP	69	29.856 -10.995	55.112	1.00 33.96	В
60	ATOM	416	С	ASP	69	33.775 -10.414	53.078	1.00 30.67	В
	MOTA	417	0	ASP	69	33.594 -10.882	51.970	1.00 31.26	В
	MOTA	418	N	MET	70	34.816 -9.646	53.377	1.00 31.20	В
	ATOM	419		MET	70	35.836 -9.294	52.394	1.00 31.00	В
		420							
65	MOTA			MET	70	35.396 -8.081	51.567	1.00 33.24	В
O)	MOTA	421		MET	70	34.253 -8.330	50.598	1.00 35.15	В
	ATOM	422		MET	70	33.994 -6.921	49.476	1.00 43.03	В
	ATOM	423	CE	MET	70	32.288 -6.531	49.777	1.00 42.27	В
	ATOM	424		MET	70	37.158 -8.978	53.090	1.00 29.72	В
	ATOM	425		MET	70	37.186 -8.682	54.271	1.00 29.23	В
70	MOTA	426		VAL	71			1.00 28.80	В
, ,							52.353		
	ATOM	427		VAL	71	39.561 -8.765	52.929	1.00 30.15	В
	MOTA	428		VAL	71	40.256 -10.054	53.443	1.00 31.84	В
	MOTA	429	CG1	VAL	71	41.603 -9.713	54.060	1.00 33.61	В

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	MOTA	430	CG2		71		-10.738	54.471	1.00 31.83	В
	MOTA	431	С	VAL	71	40.439	-8.102	51.878	1.00 29.25	В
	MOTA	432	0	VAL	71	40.471	-8.526	50.734	1.00 30.25	В
	MOTA	433	N	PHE	72	41.146	-7.053	52.285	1.00 30.15	В
5	ATOM	434	CA	PHE	72	42.015	-6.306	51.384	1.00 30.67	В
-	ATOM	435	CB	PHE	72	41.445	-4.905	51.152	1.00 28.16	В
									1.00 27.42	В
	MOTA.	436	CG	PHE	72	40.060	-4.903	50.573		
,	MOTA	437	CD1		72	39.854	-5.145	49.220	1.00 26.23	В
	MOTA	438	CD2	PHE	72	38.955	-4.686	51.390	1.00 26.64	В
10	MOTA	439	CE1	PHE	72	38.565	-5.171	48.688	1.00 25.66	В
	MOTA	440	CE2		72	37.664	-4.709	50.868	1.00 25.86	В
	MOTA	441	cz	PHE	72	37.469		49.516	1.00 24.73	В
					72		-6.188	51.940	1.00 31.84	B
	MOTA	442	C	PHE		43.428				
1.5	MOTA	443	0	PHE	72	43.646	-5.560	52.973	1.00 30.82	В
15	ATOM	444	N	GLY	73	44.385	-6.797	51.247	1.00 32.27.	В
	ATOM	445	CA	GLY	73	45.757	-6.727	51.697	1.00 32.67	В
	MOTA	446	С	GLY	73	46.358	-5.377	51.366	1.00 33.72	В
	MOTA	447	0	GLY	73	45.730	-4.553	50.707	1.00 33.21	В
	ATOM	448	N	ALA	74	47.589	-5.163	51.815	1.00 34.20	В
20	MOTA	449	CA	ALA	74	48.296	-3.911	51.583	1.00 35.80	В
20										B
	MOTA	450	CB	ALA	74	49.615	-3.929	52.329	1.00 35.10	
	MOTA	451	С	ALA	74	48.547	-3.664	50.100	1.00 37.02	В.
	MOTA	452	0	ALA	74	49.235	-2.734	49.730	1.00 38.45	В
	ATOM	453	N	SER	75	47.971	-4.498	49.250	1.00 38.40	· B
25	MOTA	454	CA	SER	75	48.179	-4.356	47.821	1.00 40.23	В
_	ATOM	455	CB	SER	75	48.437	-5.733	47.204	1.00 40.06	В
	MOTA	456	0G	SER	75	47.371	-6.617	47.504	1.00 38.50	В
	MOTA							47.126	1.00 40.71	В
		457	Ċ	SER	75	46.990	-3.701			
20	MOTA	458	0	SER	75	47.155	-3.026	46.109	1.00 40.44	В
30	MOTA	459		THR	76	45.795	-3.917	47.677	1.00 40.56	В
	MOTA	460	CA	THR	76	44.568	-3.365	47.107	1.00 40.11	В
	MOTA	461	СВ	THR	76	43.325	-3.769	47.960	1.00 41.15	. В
	ATOM	462	OG1		76	43.690	-3.865	49.342	1.00 43.22	В
	MOTA	463		THR	76	42.774	-5.118	47.498	1.00 43.01	В
35										В
23	MOTA	. 464	C	THR	76	44.615	-1.849	46.937	1.00 38.50	
•	MOTA	465	0	THR	76	45.071	-1.119	47.819	1.00 38.53	В
	MOTA	466	N	LYS	77	44.152	-1.385	45.785	1.00 36.21	В
	MOTA	467	CA	LYS	77	44.135	0.036	45.483	1.00 34.26	В
	MOTA	468	СВ	LYS	77	44.482	0.243	44.011	1.00 36.10	В
40	MOTA	469		LYS	77	45.901	-0.174	43.651	1.00 39.66	В
. •	MOTA	470		LYS	77	46.138	-0.013	42.153	1.00 43.10	В
	ATOM				77	47.538	-0.446	41.749	1.00 44.09	В
		471	CE	LYS						
	MOTA	472	NZ	LYS	77	47.693	-0.451	40.261	1.00 46.93	В
45	MOTA	473		LYS	77	42.776	0.662	45.799	1.00 32.74	В
45	MOTA	474	0	LYS	77	41.807	-0.045	46.049	1.00 30.61	В
	MOTA	475	N	GLN	78	42.729	1.994	45.800	1.00 31.08	В
	MOTA	476	CA	GLN	78	41.499	2.731	46.084	1.00 29.81	В
	MOTA	477		GLN	78	41.718	4.241	45.896	1.00 29.96	В
	MOTA	478		GLN	78	42.791	4.867	46.790	1.00 28.93	В
50									1.00 28.69	В
50	MOTA	479		GLN	78	42.339	5.029	48.224		
	MOTA	480	OE1		78	41.731	4.136	48.789	1.00 28.17	В
	MOTA	481		GLIN	78	42.647	6.177	48.822	1.00 28.63	В
	MOTA	482	С	GLN	78	40.371	2.273	45.160	1.00 29.13	В
	MOTA	483	0	GLN	78	39.255	2.045	45.597	1.00 28.04	В
55	MOTA	484	N	ILE	79	40.687	2.140	43.877	1.00 27.65	В
	MOTA	485	CA	ILE	79	39.710	1.730	42.874	1.00 28.90	В
					79			41.472		В
	MOTA	486	CB	ILE		40.369	1.664		1.00 28.34	
	MOTA	487	CG2		79	41.411	0.564	41.442	1.00 30.45	В.
<i>-</i> -	MOTA	488	CG1	ILE	79	39.316	1.396	40.400	1.00 29.43	В
60	ATOM	489	CD1	ILE	79	38.333	2.517	40.226	1.00 30.66	В
	MOTA	490	С	ILE	79	39.055	0.377	43.191	1.00 28.47	В
	MOTA	491	ŏ	ILE	79	37.867	0.175	42.938	1.00 27.79	В
	ATOM	492	N	ASP	80	39.829	-0.548	43.749	1.00 28.15	В
65	MOTA	493		ASP	80	39.296	-1.866	44.076	1.00 27.60	В
65	ATOM	494		ASP	80	40.435	-2.865	44.316	1.00 27.34	В
	MOTA	495	CG	ASP	80	41.439	-2.908	43.164	1.00 29.59	В
	MOTA	496	OD1	ASP	80	41.018	-2.784	41.987	1.00 27.17	В
	MOTA	497	OD2		80	42.648	-3.078	43.445	1.00 29.79	В
	MOTA	498	c	ASP	80	38.395	-1.800	45.303	1.00 27.71	В
70							-2.492		1.00 27.71	В
, ,	ATOM	499	0	ASP	80	37.394		45.383		
	MOTA	500		VAL	81	38.761	-0.964	46.265	1.00 28.05	. В
	MOTA	501	CA	VAL	81	37.947	-0.820	47.460	1.00 27.29	В
	MOTA	502	CB	VAL	81	38.618	0.115	48.495	1.00 25.22	В

	MOTA	503	CG1	VAL	81	37.662	0.394	49.633	1.00 21.33	В
	ATOM	504	CG2	VAL	81	39.890	-0.532	49.036	1.00 23.97	В
	MOTA	505	c	VAL	81	36.588	-0.244	47.079	1.00 28.97	В
							-0.682		1.00 29.68	В
5	ATOM	506	0	VAL	81	35.555		47.590		
J	MOTA	507	N	TYR	82	36.593	0.721	46.162	1.00 28.62	В
	ATOM	508	CA	TYR	82	35.364	1.368	45.723	1.00 30.02	В
	MOTA	509	CB	TYR	82	35.693	2.640	44.924	1.00 31.49	В
	ATOM	510	CG	TYR	82	34.472	3.389	44.443	1.00 33.00	В
	ATOM	511	CD1		82	33.934	3.144	43.180	1.00 34.00	В
10	ATOM	512	CE1		82	32.776	3.781	42.762	1.00 37.72	В
10										
	MOTA	513	CD2	TYR	82	33.817	4.299	45.278	1.00 32.60	В
	MOTA	514	CE2		82	32.659	4.938	44.871	1.00 36.04	В
	MOTA	515	cz	TYR	82	32.142	4.676	43.613	1.00 39.42	В
	ATOM	516	OH	TYR	82	30.992	5.316	43.203	1.00 42.75	В
15	MOTA	517	С	TYR	82	34.456	0.451	44.906	1.00 30.88	В
	MOTA	518	ŏ	TYR	82	33.264	0.363	45.168	1.00 30.76	В
						35.021	-0.223	43.910	1.00 32.85	В
	MOTA	519	N	ARG	83					
	MOTA	520	CA	ARG	83	34.239	-1.136	43.077	1.00 34.09	В
^^	MOTA	521	CB	ARG	83	35.120	-1.702	41.965	1.00 35.60	В
20	MOTA	522	CG	ARG	83	35.333	-0.749	40.798	1.00 42.48	В
	MOTA	523	CD	ARG	83	36.652	-1.013	40.072	1.00 46.99	В
	ATOM:	524	NE	ARG	83	36.734	-2.358	39.503	1.00 53.06	В
	ATOM	525	cz	ARG	83	36.100	-2.758	38.404	1.00 56.78	В
		526	NH1		83	35.323	-1.914	37.735	1.00 57.61	В
25	MOTA									
23	ATOM	527	NH2		83	36.254	-4.004	37.967	1.00 57.03	В
	MOTA	528	С	ARG	83	33.630	-2.277	43.895	1.00 33.36	В
	MOTA	529	0	ARG	83	32.492	-2.674	43.667	1.00 34.00	В
	MOTA	530	N	SER	84	34.390	-2.785	44.860	1.00 31.69	В
	MOTA	531	ÇA	SER	84	33.956	-3.899	45.701	1.00 30.91	В
30	MOTA	532	CB	SER	84	35.180	-4.582	46.322	1.00 31.88	В
-	ATOM	533	OG	SER	84	36.115	-4.951	45.324	1.00 34.36	В
									1.00 30.39	
	ATOM	534	C	SER	84	32.983	-3.535	46.816		В
	MOTA	535	0	SER	84	31.963	-4.195	47.007	1.00 30.60	В
	MOTA	536	N	VAL	85	33.299	-2.489	47.568	1.00 29.66	В
35	MOTA	537	CA	VAL	85	32.432	-2.091	48.663	1.00 28.01	В
	MOTA	538	СВ	VAL	85	33.255	-1.652	49.887	1.00 27.01	В
	ATOM	539	CG1		85	32.336	-1.128	50.971	1.00 26.26	В
	ATOM	540				34.080	-2.815	50.407	1.00 26.27	В
					85					
άO	MOTA	541	C	VAL	85	31.445	-0.983	48.337	1.00 27.47	В
40	ATOM	542	0	VAL	85	30.249	-1.149	48.498	1.00 28.23	В
	MOTA	543	N	VAL	86	31.960	0.145	47.868	1.00 28.02	В
	ATOM	544	CA	VAL	86	31.132	1.313	47.585	1.00 28.51	В
	MOTA	545	CB	VAL	86	32.004	2.568	47.370	1.00 26.65	В
	ATOM	546	CG1		86	31.180	3.808	47.625	1.00 25.89	В
45		547			86	33.220	2.532	48.267	1.00 25.41	В
73	ATOM									
	ATOM	548	С	VAL	86	30.150	1.224	46.425	1.00 29.30	В
	MOTA	549	0	VAL	86	28.959	1.479	46.599	1.00 28.44	В
	MOTA	550	N	CYS	87	30.649	0.881	45.244	1.00 29.85	В
	MOTA	551	CA	CYS	87	29.802	0.786	44.064	1.00 33.34	В
50	MOTA	552	CB	CYS	87	30.549	0.025	42.965	1.00 36.49	В
	ATOM	553	SG	CYS	87	29.936	0.313	41.286	1.00 43.07	В
	MOTA	554		CYS	87	28.445	0.131	44.373	1.00 34.93	B
			C							
	MOTA	555	0	CYS	87	27.396	0.670	44.026	1.00 34.18	В
	ATOM	556	N	PRO	88	28.452	-1.035	45.045	1.00 35.57	В
55	MOTA	557	CD	PRO	88	29.603	-1.876	45.420	1.00 37.48	В
	MOTA	558	CA	PRO	88	27.195	-1.715	45.378	1.00 35.50	В
	ATOM	559	CB	PRO	88	27.664	-2.989	46.078	1.00 35.52	В
	MOTA	560	CG	PRO	88	28.984	-3.247	45.464	1.00 36.85	В
	ATOM	561		PRO	88	26.295	-0.874	46.287	1.00 35.13	В
60			C							
UU	MOTA	562	0	PRO	88	25.099	-0.765	46.050	1.00 35.74	В
	MOTA	563	N	ILE	89	26.885	-0.288	47.327	1.00 34.00	В
	MOTA	564	CA	ILE	89	26.140	0.535	48.279	1.00 33.52	В
	ATOM	565	CB	ILE	89	27.031	0.978	49.465	1.00 33:84	В
	ATOM	566	CG2		89	26.250	1.910	50.384	1.00 34.73	В
65	ATOM	567	CG1		89	27.514	-0.247	50.243	1.00 33.35	. В
05										
	MOTA	568	CD1		89	28.486	0.077	51.357	1.00 33.52	В
	MOTA	569	C	ILE	89	25.552	1.786	47.636	1.00 32.98	В
	MOTA	570	0	ILE	89	24.485	2.243	48.016	1.00 33.67	В
	MOTA	571	N	LEU	90	26.258	2.341	46.662	1.00 32.32	В
70	ATOM	572	CA	LEU	90	25.782	3.540	45.996	1.00 32.57	В
	ATOM	573	СВ	LEU	90	26.866	4.097	45.074	1.00 30.54	В
	ATOM	574	CG	LEU	90	26.431	5.292	44.229	1.00 29.69	В
	MOTA	575	CD1	FEU	90	26.018	6.448	45.122	1.00 28.62	В

	MOTA	576	CD2	LEU	90	27.564	5.695	43.319	1.00 31.53	В
	MOTA	577	С	LEU	90	24.504	3.272	45.202	1.00 32.92	В
	MOTA	578	0	LEU	90	23.567	4.074	45.240	1.00 32.45	В
	MOTA	579	N	ASP	91	24.466	2.147	44.491	1.00 33.45	В
5 ·	ATOM	580	CA	ASP	91	23.292	1.785	43.699	1.00 34.72	В
,										
	MOTA	581	СВ	ASP	91	23.520	0.470	42.940	1.00 35.65	В
	ATOM	582	CG	ASP	91	24.593	0.582	41.863	1.00 39.61	В
	MOTA	583	OD1	ASP	91	24.686	1.648	41.214	1.00 40.33	В
	ATOM	584	OD2	ASP	91	25.335	-0.409	41.661	1.00 41.38	В
10	MOTA	585	C	ASP	91	22.068	1.633	44.597	1.00 33.10	В
	ATOM	586	ō	ASP	91	20.954	1.885	44.174	1.00 33.56	В
										В
	MOTA	587	N	GLU	92	22.290	1.221	45.839	1.00 32.56	
	MOTA	588	CA	GLU	92	21.196	1.044	46.783	1.00 34.16	В
	ATOM	589	CB	GLU	92	21.657	0.171	47.954	1.00 37.44	В
15	MOTA	590	CG	GLU	92	20.545	-0.258	48.890	1.00 42.74	В
	ATOM	591	CD	GLU	92	20.880	-1.536	49.648	1.00 46.50	В
	ATOM	592	OE1		92	20.053	-1.956	50.490	1.00 47.07	В
		593	OE2		92	21.962	-2.120	49.396	1.00 46.74	B
	MOTA									
20	MOTA	594	С	GLU	92	20.709	2.409	47.280	1.00 32.53	В
20	MOTA	595	0	GLU	92	19.518	2.608	47.519	1.00 30.70	В
	ATOM	596	N	VAL	93	21.641	3.348	47.422	1.00 31.20	₿
	ATOM	597	CA	VAL	93	21.303	4.699	47.854	1.00 31.28	В
	ATOM	598	CB	VAL	93	22.580	5.569	48.076	1.00 31.49	в
	ATOM	599	CG1		93	22.194	7.010	48.365	1.00 27.40	В
25									1.00 33.28	В
23	MOTA	600	CG2		93	23.398	5.004	49.233		
	MOTA	601	С	VAL	93	20.452	5.322	46.750	1.00 29.79	В
	MOTA	602	0	VAL	93	19.416	5.913	47.013	1.00 28.28	В
	ATOM	603	N	ILE	94 .	20.899	5.163	45.510	1.00 27.82	В
	MOTA	604	CA	ILE	94	20.166	5.703	44.378	1.00 30.44	В
30	MOTA	605	CB	ILE	94	20.915	5.429	43.051	1.00 28.59	В
	MOTA	606	CG2		94	20.035	5.787	41.853	1.00 26.78	В
					94		6.240	43.037	1.00 27.01	В
	ATOM	607	CG1			22.216				
	ATOM	608	CD1		94	23.087	5.978	41.846	1.00 26.60	В
20	MOTA	609	С	ILE	94	18.749	5.131	44.306	1.00 32.32	В
35	MOTA	. 610	0	ILE	94	17.872	5.738	43.714	1.00 32.23	В
	MOTA	611	N	MET	95	18.531	3.968	44.920	1.00 34.51	В
	MOTA	612	CA	MET	95	17.201	3.360	44.923	1.00 36.17	В
	ATOM	613	СВ	MET	95	17.282	1.850	45.149	1.00 38.61	В
	ATOM				95		1.017	43.881	1.00 40.44	В
40		614	CG	MET		17.372				
40	MOTA	615	SD	MET	95	17.488	-0.772	44.242	1.00 46.46	В
	MOTA	616	CE	MET	95	19.102	-1.171	43.546	1.00 44.51	В
	ATOM	617	С	MET	95	16.315	3.979	45.996	1.00 36.50	В
	MOTA	618	0	MET	95	15.113	3.732	46.030	1.00 37.42	В
	ATOM	619	N	GLY	96	16.914	4.775	46.879	1.00 36.28	В
45	ATOM	620	CA	GLY	96	16.145	5.414	47.932	1.00 35.74	В
13							4.830	49.314	1.00 36.78	В
	MOTA	621	C	GLY	96	16.366				
	ATOM	622	0	GLY	96	15.538	5.026	50.210	1.00 37.90	В
	MOTA	623	N	TYR	97	.17.479	4.118	49.487	1.00 36.85	В
	ATOM	624	CA	TYR	97	17.835	3.496	50.763	1.00 37.58	В
50	MOTA	625	CB	TYR	97	18.381	2.081	50.525	1.00 40.65	В
	MOTA	626	CG	TYR	97	17.341	1.025	50.217	1.00 45.13	В
	ATOM	627	CD1		97	16.518	0.518	51.220	1.00 46.62	В
							-0.454	50.944	1.00 49.26	В
	MOTA	628	CE1		97	15.558				
	ATOM	629	CD2		97	17.182	0.533	48.921	1.00 46.06	В
55	MOTA	630	CE2	TYR	97	16.228	-0.436	48.630	1.00 49.09	В
	MOTA	631	CZ	TYR	97	15.417	-0.928	49.546	1.00 50.42	В
	MOTA	632	ОН	TYR	97	14.465	-1.888	49.358	1.00 52.50	В
	ATOM	633	C	TYR	97	18.889	4.304	51.526	1.00 35.44	В
	ATOM	634	ŏ	TYR	97	19.789	4.876	50.926	1.00 37.02	В
60 -										
00	MOTA	635	N	ASN	98	18.776	4.349	52.849	1.00 31.97	В
	MOTA	636	CA	ASN	98	19.759	5.059		1.00 30.42	В
	MOTA	637	CB	ASN	98	19.169	5.460	55.025	1.00 30.64	В
	MOTA	638	CG	ASN	98	18.239	6.663	54.945	1.00 28.74	В
	MOTA	639		ASN	98	18.255	7.413	53.981	1.00 29.47	В
65	ATOM	640	ND2		98	17.436	6.855	55.984	1.00 27.34	В
4 3										
	MOTA	641	C	ASN	98	20.942	4.124	53.897	1.00 29.81	В
	MOTA	642	0	ASN	98	20.762	3.006	54.324	1.00 29.82	В
	MOTA	643	N	CYS	99	22.152	4.590	53.615	1.00 28.53	В
	MOTA	644	CA	CYS	99	23.339	3.767	53.816	1.00 26.90	В
70	MOTA	645	CB	CYS	99	23.974	3.384	52.477	1.00 28.87	В
	ATOM	646	SG	CYS	99	22.946	2.349	51.428	1.00 34.21	В
						24.382	4.465	54.677	1.00 25.00	В
	MOTA	647	c	CYS	99					
	MOTA	648	0	CYS	99	24.380	5.670	54.830	1.00 25.25	В

	MOTA	649	N	THR	100	25.285	3.671	55.232	1.00 23.32	В
	MOTA	650	CA	THR	100	26.341	4.187	56.080	1.00 19.59	В
	MOTA	651	CB	THR	100	25.876	4.258	57.544	1.00 17.10	В
_	MOTA	652	0G1	THR	100	24.789	5.179	57.657	1.00 16.21	В
5	MOTA	653	CG2	THR	100	27.005	4.696	58.456	1.00 15.27	В
-					100					В
	MOTA	654		THR		27.552	3.266	55.982	1.00 21.18	
	ATOM	655	0	THR	100	27.417	2.039	56.005	1.00 22.70	В
	ATOM	656		ILE	101	28.732	3.858	55.849	1.00 18.53	В
	MOTA	657	CA	ILE	101	29.967	3.097	55.782	1.00 17.55	В
10	MOTA	658	CB	ILE	101	30.650	3.212	54.420	1.00 16.14	В
10										
	MOTA	659	CG2	ILE	101	31.939	2.414	54.423	1.00 16.50	В
	MOTA	660	CG1	ILE	101	29.730	2.690	53.318	1.00 14.57	В
										В
	MOTA	661	CD1		101	30.186	3.077	51.930	1.00 14.45	
	MOTA	662	С	ILE	101	30.913	3.654	56.834	1.00 19.99	В
15	MOTA	663		ILE	101	31.296	4.822	56.786	1.00 20.78	В
	ATOM	664	N	PHE	102	31.273	2.808	57.793	1.00 19.14	В
	ATOM	665	CA	PHE	102	32.176	3.179	58.876	1.00 17.58	В
								60.123		В
	MOTA	666		PHE	102	31.835	2.373		1.00 17.67	
	MOTA	667	CG	PHE	102	30.618	2.842	60.847	1.00 17.05	В
20	MOTA	668	CD1	PHP	102	30.714	3.855	61.790	1.00 16.04	В
	ATOM	669	CD2	PHE	102	29.386	2.239	60.624	1.00 16.40	В
	MOTA	670	CE1	PHE	102	29.603	4.265	62.508	1.00 16.56	В
	MOTA	671		PHE	102	28.268	2.643	61.337	1.00 18.62	В
	MOTA	672	CZ	PHE	102	28.377	3.658	62.283	1.00 16.81	В
25	MOTA	673	С	PHE	102	33.625	2.891	58.515	1.00 16.69	В
	MOTA	674	0	PHE	102	33.910	2.289	57.516	1.00 18.17	. В
	MOTA	675	N	ALA	103	34.535	3.338	59.366	1.00 17.68	В
	MOTA	676		ALA	103	35.961	3.089	59.187	1.00 17.02	В
••	MOTA	677	CB	ALA	103	36.620	4.229	58.451	1.00 16.82	В
30	MOTA	678	С	ALA	103	36.471	2.991	60.617	1.00 17.64	В
				ALA						
	MOTA	679			103	36.482	3.963	61.339	1.00 18.79	В
	MOTA	680	N	TYR	104	36.866	1.786	61.012	1.00 18.22	В
	MOTA	681	CA	TYR	104	37.340	1.540	62.368	1.00 16.40	В
0.5	MOTA	682	CB	TYR	104	36.436	0.496	63.034	1.00 15.83	В
35	MOTA	683	CG	TYR	104	36.706	0.291	64.508	1.00 12.67	В
	MOTA	684	CD1					64.941		В
					104	37.771	-0.501		1.00 10.95	
	MOTA	685	CEl	TYR	104	38.046	-0.659	66.301	1.00 11.52	В
	MOTA	686	CD2	TYR	104	35.919	0.920	65.469	1.00 10.91	В
40	MOTA	687	CE2	TYR	104	36.187	0.768	66.832	1.00 12.42	В
40	MOTA	688	CZ	TYR	104	37.253	-0.023	67.239	1.00 10.32	В
		689		TYR				68.574		В
	MOTA				104	37.526	-0.180		1.00 11.99	
	ATOM	690	С	TYR	104	38.778	1.061	62.380	1.00 15.64	В
	MOTA	691	- 0	TYR	104	39.203	0.348	61.497	1.00 17.51	В
40	MOTA	692	N	GLY	105	39.524	1.456	63.397.	1.00 15.78	В
45	MOTA	693	CA	GLY	105	40.904	1.047	63.475	1.00 16.05	В
	ATOM	694		GLY	105	41.748	2.044	64.226	1.00 16.81	В
	MOTA	695	0	GLY	105	41.318	3.151	64.526	1.00 19.22	В
	MOTA	696	N	GLN	106	42.963	1.616	64.531	1.00 18.16	B
	MOTA	697		GLN	106					В
50						43.940	2.408	65.244	1.00 18.74	
50	ATOM	698	CB	GLN	106	45.122	1.519	65.652	1.00 19.69	B
	MOTA	699	CG	GLN	106	46.278	2.251	66.305	1.00 23.87	В
	MOTA	700		GLN	106	47.527	1.411	66.407	1.00 24.14	В
	MOTA	701	OE1	GLN	106	47.865	0.669	65.490	1.00 27.37	В
	MOTA	702	NE2	CLN	106	48.225	1.528	67.525	1.00 25.29	В
55										
JJ	MOTA	703	C	GLN	106	44.440	3.552	64.363	1.00 20.10	В
	MOTA	704	0	GLN	106	44.438	3.451	63.134	1.00 19.09	В
	MOTA	705		THR	107				1.00 19.11	В
						44.864	4.639	65.004		
	MOTA	706	CA '	THR	107	45.385	5.792	64.291	1.00 18.65	В
	MOTA	707		THR	107	45.849	6.914	65.270	1.00 20.97	В
60										
JU	MOTA	708	OG1		107	44.730	7.405	66.017	1.00 19.66	В
	MOTA	709	CG2	THR	107	46.476	8.064	64.497	1.00 15.96	В
	MOTA	710		THR	107	46.588	5.391	63.439	1.00 17.71	В
	MOTA	711	0	THR	107	47.518	4.747	63.921	1.00 16.56	B
	MOTA	712		GLY	108	46.554	5.786	62.171	1.00 17.28	В
65										
0.5	MOTA	713		GĻY	108	47.642	5.483	61.267	1.00 15.71	В
	MOTA	714	C	GLY	108	47.499	4.181	60.505	1.00 17.55	В
	MOTA	715		GLY				59.938	1.00 17.87	В
					108	48.489	3.682			
	MOTA	716	N '	THR	109	46.288	3.626	60.478	1.00 15.83	В
	MOTA	717		THR	109	46.064	2.374	59.765	1.00 14.74	В
70										
<i>,</i> 0	MOTA	718		THR	109	45.276	1.352	60.632	1.00 13.57	₿
	ATOM	719	OG1 '	THR	109	43.978	1.866	60.943	1.00 13.63	В
	ATOM	720	CG2						1.00 12.00	В
					109	46.035	1.064	61.934		
	MOTA	721	C '	THR	109	45.350	2.573	58.435	1.00 15.88	В

	•									
	MOTA	722	0	THR	109	45.132	1.602	57.708	1.00 14.55	В
			0	Inn						
	ATOM	723	N	GLY	110	44.977	3.819	58.124	1.00 13.70	В
	ATOM	724	CA	GLY	110	44.321	4.073	56.849	1.00 10.56	В
	MOTA	725	С	GLY	110	42.846	4.433	56.833	1.00 10.76	В
_								-		
5	MOTA	726	0	GLY	110	42.201	4.298	55.792	1.00 9.95	В
										В
	MOTA	727	N	LYS	111	42.302	4.885	57.959	1.00 8.99	
	MOTA	728	CA	LYS	111	40.889	5.267	58.022	1.00 11.48	В
	MOTA	729	CB	LYS	111	40.497	5.693	59.449	1.00 12.59	В
	MOTA	730	CG	LYS	111	40.315	4.531	60.426	1.00 15.28	В
10	MOTA	731	CD	TVC	3 7 1	39.651	4.955	61.738	1.00 12.73	В
10				LYS	111					
	MOTA	732	CE	LYS	111	40.439	6.034	62.455	1.00 11.56	B
	MOTA	733	NZ	LYS	111	41.905	5.766	62.396	1.00 10.51	В
	MOTA	734	С	LYS	111	40.575	6.408	57.062	1.00 13.97	В
	AION		_		111					
	MOTA	735	0	LYS	111	39.683	6.302	56.206	1.00 15.37	В
15										
15	ATOM	736	N	THR	112	41.321	7.498	57.198	1.00 13.82	В
	MOTA	737	CA	THR	112	41.120	8.663	56.353	1.00 12.58	В
	MOTA	738	CB	THR	112	41.895	9.871	56.926	1.00 12.79	В
						41.408				
	ATOM	739		THR	112	41.400	10.160	58.245	1.00 9.63	В
	ATOM	740	CG2	THR	112	41.723	11.103	56.037	1.00 10.46	В
20										
20	MOTA	741	С	THR	112	41.535	8.396	54.905	1.00 14.40	В
	MOTA	742	0	THR	112	40.886	8.846	53.978	1.00 15.19	В
	ATOM	743	N	PHE	113	42.618	7.651	54.723	1.00 15.74	₿.
	MOTA	744	CA	PHE	113	43.095	7.326	53.384	1.00 17.09	В
	MOTA	745	CB	PHE	113	44.316	6.408	53.463	1.00 17.69	·B
25										
43	MOTA	746	CG	PHE	113	44.867	6.030	52.123	1.00 20.87	В
	MOTA	747	CDI	PHE	113	45.783	6.849	51.475	1.00 22.41	В
	MOTA	748	CD2	PHE	113	44.445	4.871	51.490	1.00 22.63	В
	MOTA	749	CEI	PHE	113	. 46:271	6.517	50.218	1.00 22.81	В
	MOTA	750	CE2	PHE	113	44.924	4.529	50.228	1.00 23.87	В
20										
30	ATOM	751	CZ	PHE	113	45.840	5.354	49.590	1.00 25.27	В
							c cac			
	MOTA	752	С	PHE	113	42.000	6.626	52.580	1.00 18.62	В
	MOTA	753	0	PHE	113	41.817	6.888	51.389	1.00 17.60	В
	MOTA	754	N	THR	114	41.291	5.719	53.247	1.00 19.63	В
		755	CA	THE		40.212	4.945	52.646	1.00 18.57	В
25	MOTA		CA	THR	114					
35	MOTA	· 756	CB	THR	114	39.816	3.760	53.582	1.00 20.30	B
	MOTA	757	OGI	THR	114	40.970	2.947	53.828	1.00 18.79	В
	MOTA	758	CG2	THR	114	38.700	2.910	52.972	1.00 12.74	B
	MOTA	759	С	THR	114	38.991	5.825	52.410	1.00 19.70	В
							E 022		3 00 22 32	
40	MOTA	760	۰0	THR	114	38.497	5.932	51.297	1.00 22.13	В
40	MOTA	761	N	MET	115	38.518	6.473	53.465	1.00 19.43	В
. •										
	ATOM	762	CA	MET	115	37.345	7.318	53.347	1.00 20.55	В
	N TO M	763	CB	MET	115	36.877	7.771	54.730	1.00 21.97	В
	MOTA									
	ATOM	764	CG	MET	115	36.471	6.620	55.644	1.00 27.07	В
	ATOM	765	SD	MET	115	35.328	5.432	54.848	1.00 29.66	В
45	MOTA	766	CE	MET	115	33.753	6.265	55.089	1.00 27.98	В
	MOTA	767	С	MET	115	37.532	8.528	52.454	1.00 21.26	В
	MOTA	768	0	MET	115	36.639	8.866	51.674	1.00 23.74	В
	ATOM	769	N	GLU	116	38.687	9.179	52.549	1.00 20.10	В
	ATOM	770	CA.	GLU	116	38.937	10.377	51.749	1.00 20.30	В
50	MOTA	771	CB	GLU	116	39.323	11.541	52.659	1.00 19.03	В
	ATOM	772	CG	GLU	116	38.309	11.824	53.741	1.00 17.09	В
	MOTA	773	CD	GLU	116	38.746	12.922	54.687	1.00 18.90	В
	ATOM	774	OEl	GLU	116	39.886	13.421	54.550	1.00 21.39	В
	ATOM	775	OEZ	GLU	116	37.951	13.280	55.579	1.00 17.52	В
55	MOTA	776	C·	GLU	116	40.010	10.194	50.694	1.00 20.60	В
-										
	MOTA	777	0	GLU	116	39.804	10.494	49.527	1.00 19.26	В
			N							
•	MOTA	778		GLY	117	41.166	9.708	51.116	1.00 22.39	В
	MOTA	779	CA	GLY	117	42.249	9.508	50.176	1.00 24.67	В
	ATOM	780	C	GLY	117	43.194	10.689	50.144	1.00 25.76	В
60	ATOM	781	0							В
00				GLY	117	43.056	11.630	50.918	1.00 24.17	
	ATOM	782	N	GLU	118	44.162	10.635	49.237	1.00 27.49	В
	MOTA	783	CA	GLU	118	45.133	11.710	49.128	1.00 28.73	В
	ATOM	784	CB	GLU	118	46.465	11.273	49.740	1.00 30.64	В
	MOTA	785	CG	GLU	118	46.311	10.255	50.853	1.00 35.23	В
65										
$\sigma_{\mathcal{I}}$	MOTA	786	CD	GLU	118	47.579	10.060	51.657	1.00 37.43	В
	ATOM	787	OE1	GLU	118	48.671	9.993	51.049	1.00 35.58	В
	MOTA	788	OE2	GLU	118	47.476	9.958	52.900	1.00 40.04	В
	ATOM	789	С	GLU	118	45.338	12.082	47.671	1.00 27.97	В
	MOTA	790	0	GLU	118	44.692	11.542	46.779	1.00 29.50	В
70										
70	ATOM	791	N	ARG	119	46.244	13.017	47.436	1.00 25.87	В
	ATOM	792	ÇA							В
				ARG	119	46.532	13.439	46.085	1.00 25.52	
	ATOM	793	CB.	ARG	119	46.613	14.968	46.006	1.00 24.48	В
	ATOM	794	CG	ARG	119	45.323	15.708	46.358	1.00 23.62	В

	ATOM	795	CD	ARG	119	44.190	15.361	45.387	1.00 22.16	В
	ATOM	796	NE	ARG	119	44.654	15.191	44.011	1.00 20.25	В
	MOTA	797	CZ	ARG	119	44.382	16.018	43.005	1.00 19.31	В
_	ATOM	798	NH1	ARG	119	43.642	17.102	43.203	1.00 19.24	В
5	ATOM	799	NH2	ARG	119	44.842	15.744	41.791	1.00 17.50	В
	ATOM	800	С	ARG	119	47.857	12.836	45.654	1.00 26.80	`B
	MOTA	801	0	ARG	119	48.779	12.711	46.457	1.00 25.89	В
	MOTA	802	N	SER	120	47.942	12.440	44.390	1.00 25.98	В
	MOTA	803	CA	SER	120	49.189	11.893	43.880	1.00 28.78	В
10	ATOM	804	CB	SER	120	49.015	11.326	42.472	1.00 29.79	В
	ATOM	805	OG	SER	120	48.428	10.038	42.508	1.00 33.26	В
	MOTA	806	С	SER	120	50.130	13.077	43.834	1.00 27.18	В
	MOTA	807	0	SER	120 -	49.779	14.121	43.326	1.00 27.97	В
	MOTA	808	N	PRO	121	51.348	12.913	44.357	1.00 27.06	В
15	MOTA	809	CD	PRO	121	51.902	11.662	44.900	1.00 26.17	В
	MOTA	810	CA	PRO	121	52.350	13.987	44.381	1.00 27.66	В
	MOTA	811	CB	PRO	121	53.528	13.342	45.117	1.00 27.55	В
	MOTA	812	CG	PRO	121	53.386	11.899	44.779	1.00 28.94	В
20	HOTA	813	C	PRO	121	52.760	14.591	43.031	1.00 27.47	В
20	ATOM	814	0	PRO	121	52.773	13.914	42.009	1.00 27.14	В
	MOTA	815	N	ASN		53.072	15.885	43.050	1.00 27.34	В
	ATOM	816	CA	ASN	122	53.517	16.615	41.865.		В
	ATOM	817	CB	ASN	122	54.690	15.875	41.217	1.00 29.21	В
25	MOTA	818	CG	ASN	122	55.857	16.789	40.906	1.00 29.30	В
23	MOTA	819		ASN	122	56.355	17.491	41.777	1.00 30.37	В
	MOTA	820		ASN	122	56.305	16.774	39.656	1.00 30.61	В
	ATOM	821		ASN	122	52.434	16.859	40.817	1.00 28.67	В
	MOTA	822	0	ASN	122	52.725	16.940	39.627	1.00 25.87	В
30	ATOM	823	N	GLU	123	51.191	16.985	41.265	1.00 30.12	В
50	MOTA MOTA	824 825	CA	GLU	123	50.070	17.240 18.699	40.356	1.00 33.32	В
	ATOM	826	CB	GLU	123 123	50.105		39.870	1.00 33.54	В
	MOTA	827	CD	GLU	123	50.037 49.872	19.748 21.158	40.968 40.420	1.00 33.76	B B
•	ATOM	828		GLU	123	50.763	21.623	39.678	1.00 32.71	В
35	ATOM	829		GLU	123	48.848	21.804	40.734	1.00 33.32	В
00	MOTA	830	C	GLU	123	50.061	16.307	39.137	1.00 34.30	В
	ATOM	831	ŏ	GLU	123	49.856	16.743	38.013	1.00 32.10	В
	ATOM	832	N	GLU	124	50.283	15.020	39.373	1.00 36.35	В
	ATON	833	CA	GLU	124	50.303	14.046	38.292	1.00 36.52	В
40	ATOM	834	CB	GLU	124	50.709	12.678	38.846	1.00 40.35	В
	ATOM	835	CG	GLU	124	51.279	11.711	37.815	1.00 45.05	В
	ATOM	836	CD	GLU	124	52.026	10.550	38.458	1.00 47.77	В
	ATOM	837	OE1		124	51.966	10.427	39.705	1.00 47.83	В
	ATOM	838	OE2		124	52-671	9.769	37.720	1.00 48.04	·B
45	ATOM	839	С	GLU	124	48.942	13.964	37.590	1.00 36.15	В
	MOTA	840	0	GLU	124	48.876	13.987	36.363	1.00 34.16	В
	MOTA	841	N	TYR	125	47.859	13.886	38.361	1.00 35.31	В
	MOTA	842	CA	TYR	125	46.524	13.803	37.770	1.00 36.12	В
50	MOTA	843	CB	TYR	125	45.863	12.440	38.054	1.00 38.61	В
50	MOTA	844	CC	TYR	125	46.757	11.216	37.992	1.00 39.31	В
	MOTA	845	CD1	TYR	125	47.657	10.933	39.019	1.00 39.77	В
	MOTA	846		TYR	125	48.454	9.784	38.987	1.00 40.96	В
	MOTA	847		TYR	125	46.675	10.321	36.922	1.00 39.64	В
66	MOTA	848		TYR	125	47.468	9.169	36.879	1.00 40.42	В
55	MOTA	849	CZ	TYR	125	48.355	8.908	37.916	1.00 41.60	B
	MOTA	850	ОН	TYR		49.141	7.776	37.882	1.00 43.64	В
	MOTA	851	С	TYR	125	45.590	14.873	38.332	1.00 35.75	В
	MOTA	852	0	TYR	125	45.925	15.577	39.273	1.00 36.04	В
۲n ·	MOTA	853		THR	126	44.409	14.976	37.729	1.00 35.01	В
60	ATOM	854		THR	126	43.385	15.901	38.189	1.00 34.12	В
	MOTA	855	CB		126	42.393	16.275	37.064	1.00 34.09	В
	MOTA	856	OG1		126	41.885	15.080	36.458	1.00 36.33	В
	ATOM	857	CG2		126	43.075	17.134	36.005	1.00 30.16	В
65	MOTA	858		THR	126	42.645	15.117	39.271	1.00 34.15	. В
03	ATOM	859		THR	126	42.555	13.896	39.197	1.00 35.30	В
	ATOM	860		TRP	127	42.111	15.807	40.270	1.00 33.25	В
	MOTA	861		TRP	127	41.422	15.133	41.363	1.00 31.64	В
	MOTA	862		TRP	127	40.596	16.135	42.182	1.00 28.58	В
70	MOTA	863		TRP	127	39.362	16.610	41.489	1.00 25.55	В
70	MOTA	864	CD2		127	38.066	16.008	41.551	1.00 23.28	В
	MOTA	865	CEZ		127	37.218	16.754	40.699	1.00 23.64	В
	MOTA	866	CE3		127	37.537	14.907	42.244	1.00 23.43	В
	MOTA	867	CD1	IKP	127	39.255	17.667	40.631	1.00 23.80	В

	MOTA	868	NE1	TRP	127	37.969	17.761	40.150	1.00 24.71	В
	MOTA	869	CZ2 '	TRP	127	35.867	16.433	40.518	1.00 24.05	В
	MOTA	870		TRP	127	36.192	14.585	42.065	1.00 24.74	В
5	MOTA	871	CH2	-	127	35.372	15.351	41.207	1.00 26.04	В
5	MOTA	872		TRP	127	40.522	13.968	40.931	1.00 31.94	В
	MOTA	873		TRP	127	40.510	12.927	41.579	1.00 32.64	В
	ATOM	874 875		GLU	128	39.781	14.131	39.838	1.00 32.66	B
	MOTA MOTA	876		GLU GLU	128 128	38.869 37.785	13.078 13.669	39.394 38.502	1.00 34.68	В
10	MOTA	877		GLU	128	38.287	14.201	37.178	1.00 39.01	В
10	MOTA	878		GLU	128	37.206	14.964	36.442	1.00 42.74	B
	ATOM	879	OE1		128	36.895	16.100	36.867	1.00 44.33	В
	MOTA	880	0E2 (128	36.654	14.422	35.458	1.00 43.63	В
	MOTA	881	C	GLU	128	39.512	11.879	38.700	1.00 32.67	В
15	MOTA	882		GLU	128	38.825	10.930	38.348	1.00 31.45	В
	MOTA	883		GLU	129	40.825	11.926	38.500	1.00 32.62	В
	ATOM	884		GLU	129	41.532	10.815	37.871	1.00 33.28	В
	MOTA MOTA	885 886		GLU GLU	129 129	42.192 41.218	11.246 11.496	36.561 35.420	1.00 35.75	B B
20	MOTA	887		GLU	129	41.922	11.680	34.082	1.00 42.49	В
	MOTA	388	OE1		129	41.266	12.139	33.119	1.00 43.56	B
	ATOM	889	OE2		129	43.129	11.367	33.996	1.00 45.44	В
	ATOM	890		GLU	129	42.602	10.280	38.808	1.00 33.23	В.
0.5	MOTA	891	0 (GLU	129	43.242	9.297	38.511	1.00 33.33	·B
25	MOTA	892		ASP	130	42.776	10.934	39.951	1.00 32.98	В
	MOTA	893		ASP	130	43.789	10.516	40.912	1.00 32.86	В
	ATOM	894		ASP	130	43.884	11.544	42.045	1.00 34.15	В
	ATOM	895 896		ASP	130	45:247	11.564	42.699	1.00 35.32	B B
30	MOTA MOTA	897	OD1		130 130	45.765 45.801	10.477	43.030 42.882	1.00 36.91	В
50	ATOM	898		ASP	130	43.468	9.129	41.485	1.00 33.07	В
	ATOM	899		ASP	130	42.429	8.928	42.114	1.00 32.52	В
	ATOM	900		PRO	131	44.367	8.152	41.268	1.00 32.43	В
~~	MOTA	901	CD :	PRO	131	45.638	8.278	40.533	1.00 32.63	В
35 ·	MOTA	. 902		PRO	131	44.186	6.782	41.757	1.00 30.77	В
	MOTA	903		PRO	131	45.339	6.029	41.102	1.00 31.15	В
	MOTA	904		PRO	131	46.399	7.073	41.005	1.00 31.37	В
	MOTA	905		PRO	131	44.192	6.673	43.283	1.00 30.54	В
40	MOTA MOTA	906 907		PRO LEU	131 132	43.717 44.721	5.688 7.691	43.845 43.953	1.00 31.07 1.00 28.68	B B
70	MOTA	908		LEU	132	44.750	7.684	45.407	1.00 26.49	В
	MOTA	909		LEU	132	45.965	8.461	45.918	1.00 24.68	В
	ATOM	910		LEU	132	47.355	7.961	45.497	1.00 25.57	В
	MOTA	911	CD1	LEU	132	48.414	8.782	46.221	1.00 24.29	B
45	MOTA	912	CD2		132	47.526	6.481	45.843	1.00 26.94	В
	MOTA	913		LEU	132	43.455	8.248	46.008	1.00 26.30	В
	MOTA	914		LEU	132	43.294	8.285	47.228	1.00 26.84	В
	MOTA	915		ALA	133	42.532	8.672	45.145	1.00 24.55	В
50	MOTA MOTA	916 917		ALA ALA	133 133	41.243 40.393	9.217 9.562	45.572 44.352	1.00 25.15	B B
J	MOTA	918		ALA	133	40.502	8.215	46.453	1.00 25.64	В
	ATOM	919		ALA	133	40.528	7.034	46.201	1.00 27.86	В
	MOTA	920		GLY	134	39.831	8.706	47.485	1.00 26.27	В
	MOTA	921		GLY	134	39.107	7.822	48.379	1.00 24.63	В
55	MOTA	922		GLY	134	37.633	7.705	48.038	1.00 24.63	В
	ATOM	923		GLY	134	37.176	8.224	47.013	1.00 23.91	В
	MOTA	924		ILE	135	36.887	7.030	48.910	1.00 22.69	В
	MOTA	925		ILE	135	35.457	6.816	48.704	1.00 21.86	В
60	MOTA MOTA	926 927	CB I	ILE	135 135	34.839	5.028 5.945	49.898 49.745	1.00 21.68	B B
00	MOTA	928	CG1		135	33:315 35.464	4.628	49.971	1.00 20.31	В
	MOTA	929	CD1		135	35.183	3.865	51.246	1.00 16.89	В
	MOTA	930		ILE	135	34.652	8.103	48.481	1.00 20.87	В
	MOTA	931		ILE	135	33.956	8.228	47.495	1.00 19.45	В
65	MOTA	932	N I	ILE	136	34.762	9.053	49.405	1.00 20.74	В
	MOTA	933	CA I	ILE	136	34.018	10.309	49.297	1.00 19.78	В
	MOTA	934		ILE	136	34.420	11.273	50.436	1.00 19.46	В
•	MOTA	935	CG2		136	33.654	12.581	50.302	1.00 23.46	В
70	MOTA	936	CGI		136	34.128	10.616	51.792	1.00 19.18	В
, 0	MOTA	937	CD1		136	34.597	11.398	53.011	1.00 20.13	В
	MOTA MOTA	93B 939		ILE ILE	136 136	34.146 33.149	11.016 11.258	47.929 47.255	1.00 19.32	B B
	ATOM	940		PRO	137	35.377	11.340	47.499	1.00 18.78	В
						55.57.				_

	MOTA	941	CD	PRO	137	36.695	11.158	48.127	1.00 15.47	В
	ATOM	942	CA	PRO	137	35.501	12.008	46.198	1.00 17.79	В
					137	36.995	12.321	46.105	1.00 15.58	В
	ATOM	943	CB	PRO				46.946	1.00 16.71	В
-	MOTA	944	cc .	PRO	137	37.618	11.255			
5	MOTA	945	С	PRO	137	35.010	11.135	45.040	1.00 20.22	В
	MOTA	946	0	PRO	137	34.434	11.625	44.080	1.00 21.41	В
	MOTA	947	N	ARG	138	35.234	9.829	45.135	1.00 22.72	В
	MOTA	948	CA	ARG	138	34.789	8.927	44.075	1.00 22.41	В
				ARG	138	35.378	7.534	44.270	1.00 21.69	В
10	ATOM	949	CB						1.00 20.35	В
10	MOTA	950	CC	ARG	138	36.860	7.433	43.951		
	MOTA	951	CD	ARG	138	37.395	6.072	44.347	1.00 17.89	В
	ATOM	952	NE	ARG	138	38.847	6.020	44.275	1.00 17.83	В
	MOTA	953	CZ	ARG	138	39.529	5.905	43.142	1.00 18.07	В
	ATOM	954	NH1		138	38.886	5.818	41.987	1.00 19.38	В
15			NH2		138	40.854	5.906	43.156	1.00 18.54	В
1)	MOTA	955						44.007	1.00 22.14	В
	MOTA	956	С	ARG	138	33.263	8.829			
	MOTA	957	0	arg	138	32.689	8.890	42.942	1.00 23.68	В
	ATOM	958	N	THR	139	32.615	8.678	45.154	1.00 22.12	В
	ATOM	959	CA	THR	139	31.161	8.566	45.203	1.00 25.57	В
20	ATOM	960	СВ	THR	139	30.675	8.360	46.662	1.00 25.67	В
20			0G1		139	31.355	7.236	47.234	1.00 27.07	В
	ATOM	961						46.700	1.00 27.35	В
	ATOM	962	CG2		139	29.174	8.100			В
	MOTA	963	С	THR	139	30.463	9.797	44.614	1.00 26.55	
	MOTA	964	0	THR	139	29.544	9.675	43.809	1.00 26.69	В
25	ATOM	965	N	LEU	140	30.910	10.982	45.017	1.00 27.11	В
	ATOM	966	CA	LEU	140	30.314	12.213	44.523	1.00 26.17	В
	ATOM	967	CB	LEU	140	30.949	13.424	45.209	1.00 26.20	В
					140	30.599	13.605	46.690	1.00 26.65	В
	MOTA	968	CC	LEU				47.280	1.00 25.28	В
20	MOTA	969		LEU	140	31.435	14.723			В
30	MOTA	970	CD2	LEU	140	29.114	13.896	46.849	1.00 24.93	
	MOTA	971	С	LEU	140	30.473	12.320	43.018	1.00 25.73	В
	MOTA	972	0	LEU	140	29.556	12.725	42.333	1.00 25.93	В
	MOTA	973	N	HIS	141	31.641	11.941	42.514	1.00 25.67	В
		974	CA	HIS	141	31.907	12.001	41.081	1.00 26.55	В
35	MOTA					33.394	11.743	40.813	1.00 25.96	В
22	MOTA	975	CB	HIS	141					В
	MOTA	976	CC	HIS	141	33.770	11.804	39.364	1.00 26.57	
	ATOM	977	CD2	HIS	141	33.823	10.841	38.415	1.00 28.59	В
	MOTA	978	ND1	HIS	141	34.138	12.974	38.739	1.00 29.67	В
	ATOM	979	CE1	HIS	141	34.405	12.731	37.467	1.00 29.67	В
40	ATOM	980		HIS	141	34.221	11.443	37.245	1.00 28.28	В
	ATOM	981	c	HIS	141	31.072	10.973	40.322	1.00 26.86	В
					141	30.679	11.199	39.181	1.00 28.03	В
	ATOM	982	0	HIS					1.00 24.80	В
	MOTA	983	N	GLN	142	30.802	9.844	40.965		
	MOTA	984	CA	GLN	142	30.045	8.780	40.326	1.00 25.14	В
45	MOTA	985	CB	GLN	142	30.353	7.436	40.994	1.00 27.48	В
	MOTA	986	CG	GLN	142	31.680	6.834	40.563	1.00 30.52	В
	MOTA	987	CD	GLN	142	31.684	6.417	39.102	1.00 34.29	В
	ATOM	988		GLN	142	30.990	5.475	38.711	1.00 34.96	В
		989		GLN	142	32.468	7.116	38.287	1.00 35.49	В
50	MOTA							40.317	1.00 22.70	В
50,	MOTA	990	C	GLN	142	28.550	9.017			В
	MOTA	991	0	GLN	142	27.856	8.528	39.440	1.00 21.46	
	MOTA	992	N	ILE	143	28.058	9.766	41.297	1.00 21.92	В
	ATOM	. 993	CA	ILE	143	26.634	10.062	41.365	1.00 22.81	В
	ATOM	994	CB	ILE	143	26.304	10.888	42.620	1.00 22.20	В
55	ATOM	995	.CG2	ILE	143	24.880	11.423	42.533	1.00 22.62	В
20		996		ILE	143	26.476	10.024	43.872	1.00 21.94	В
	ATOM								1.00 20.22	В
	MOTA	997		ILE	143	26.390	10.793	45.177		
	MOTA	998	С	ILE	143	26.187	10.824	40.114	1.00 24.31	В
	MOTA	999	0	ILE	143	25.156	10.525	39.544	1.00 24.61	В
60	ATOM	1000	N	PHE	144	26.987	11.803	39.693	1.00 26.83	В
	ATOM	1001	CA	PHE	144	26.672	12.611	38.511	1.00 28.06	В
		1002	CB	PHE	144	27.580	13.857	38.439	1.00 26.87	В
	MOTA							39.536	1.00 27.89	В
	MOTA	1003	CC	PHE	144	27.330	14.861			
	MOTA	1004		PHE	144	26.169	15.630	39.545	1.00 29.48	В.
65	ATOM	1005		PHE	144	28.230	15.002	40.592	1.00 28.77	В
	ATOM	1006	CE1	PHE	144	25.901	16.518	40.592	1.00 28.27	В
	ATOM	1007		PHE	144	27.974	15.890	41.647	1.00 28.13	В
	ATOM	1008	cz	PHE	144	26.805	16.646	41.646	1.00 30.04	В
				PHE	144	26.818	11.778	37.238	1.00 28.29	В
70	MOTA	1009	c						1.00 28.71	. в
70	ATOM	1010	0	PHE	144	26.140	.12.025	36.253		
	ATOM	1011	N	GLU	145	27.703	10.786	37.273	1.00 29.40	₽
	ATOM	1012	CA	GLU	145	27.915	9.909	36.122	1.00 31.01	В
	MOTA	1013	СВ	GLU	145	29.216	9.129	36.297	1.00 32.65	В

	ATOM	1014	CC	GLU	145	30.467	9.938	36.056	1.00 38.99	В
	MOTA	1015	CD	GLU	145	30.706	10.197	34.578	1.00 43.44	В
	MOTA	1016	0E1	GLU	145	31.623	10.987	34.246	1.00 45.83	В
	MOTA	1017	OE2	CIJI	145	29.977	9.603	33.752	1.00 45.50	В
5 ·										
,	MOTA	1018	С	GLU	145	26.753	8.926	35.940	1.00 31.44	В
	MOTA	1019	0	GLU	145	26.237	8.754	34.841	1.00 30.51	В
	MOTA	1020	N	LYS	146	26.348	8.290	37.033	1.00 31.75	В
		1021								
	ATOM		CA	LYS	146	25.269	7.310	37.012	1.00 33.61	В
	MOTA	1022	CB	LYS	146	25.172	6.629	38.3B1	1.00 34.03	В
10	MOTA	1023	CG	LYS	146	26.350	5.717	38.695	1.00 38.09	В
	ATOM	1024	, CD	LYS	146	26.243	5.107	40.086	1.00 40.00	В
	MOTA	1025	CE	LYS	146	27.228	3.958	40.263	1.00 43.91	В
	ATOM	1026	NZ	LYS	146	26.919	2.818	39.352	1.00 43.76	В
	MOTA	1027		LYS	146			36.624	1.00 33.97	В
16			С			23.908	7.882			
15	MOTA	1028	0	LYS	146	23.171	7.276	35.840	1.00 33.52	В
	MOTA	1029	N	LEU	147	23.577	9.046	37.176	1.00 33.52	В
	ATOM	1030	CA	LEU	147	22.302	9.689	36.892	1.00 32.92	В
	MOTA	1031	CB	LEU	147	21.746	10.320	38.175	1.00 31.38	В
	MOTA	1032	CG	LEU	147	21.336	9.359	39.302	1.00 32.23	В
20	MOTA	1033	CD1		147	21.060	10.138	40.585	1.00 31.01	В
	MOTA	1034	CD2		147	20.096	8.569	38.883	1.00 32.23	В
	MOTA	1035	С	LEU	147	22.418	10.749	35.794	1.00 32.85	В
	MOTA	1036	0	LEU	147	21.562	11.609	35.669	.1.00 33.29	В
				THR				34.992	1.00 33.48	.в
25	MOTA	1037	N		148	23.475	10.666			
25	MOTA	1038	CA	THR	148	23.701	11.636	33.921	1.00 35.96	В
	MOTA	1039	CB	THR	148	24.900	11.236	33.036	1.00 36.22	В
	MOTA	1040	OG1		148	25.074	12.218	32.008	1.00 37.20	В
	MOTA	1041	CG2		148	24:664	9.871	32.381	1.00 38.66	В
	MOTA	1042	С	THR	148	22.484	11.879	33.014	1.00 36.52	В
30	MOTA	1043	0	THR	148	22.123	13.021	32.772	1.00 35.06	В
	MOTA	1044	N	ASP	149	21.868	10.806	32.514	1.00 35.79	В
	ATOM	1045	CA	ASP	149	20.690	10.923	31.648	1.00 35.29	В
	MOTA	1046	CB	ASP	149	21.101	11.265	30.206	1.00 36.06	В
	ATOM	1047		ASP			10.249	29.607	1.00 37.80	В
35.			CG		149	22.065				
2)	MOTA	.1048	OD1	ASP	149	22.292	9.196	30.243	1.00 40.41	В
	MOTA	1049	OD2	ASP	149	22.590	10.500	28.496	1.00 36.11	В
	MOTA	1050	С	ASP	149	19.821	9.657	31.646	1.00 34.60	В
	MOTA	1051	0	ASP	149	19.397	9.184	30.592	1.00 31.15	В
	MOTA	1052	N	asn	150	19.554	9.122	32.834	1.00 34.29	В
40	MOTA	1053	CA	ASN	150	18.732	7.923	32.948	1.00 35.52	В
. •										В
	MOTA	1054	CB	ASN	150	19.227	7.041	34.102	1.00 32.56	
	ATOM	1055	CG	ASN	150	19.031	7.690	35.452	1.00 32.34	В
	ATOM	1056	OD1	ASN	150	19.134	8.903	35.579	1.00 29.46	В
	ATOM	1057	ND2		150	18.760	6.877	36.475	1.00 31.14	В
45										
T)	MOTA	1058	С	asn	150	17.265	8.292	33.154	1.00 36.96	В
	MOTA	1059	0	ASN	150	16.436	7.431	33.447	1.00 37.74	В
	MOTA	1060	N	GLY	151	16.953	9.578	32.996	1.00 37.37	В
	ATOM	1061		GLY	151	15.585	10.044	33.153	1.00 37.75	В
	ATOM	1062	С	GLY	151	15.195	10.351	34.585	1.00 39.12	В
50	MOTA	1063	0	GLY	151	14.013	10.490	34.903	1.00 39.41	В
	MOTA	1064	N	THR	152	16.190	10.455	35.455	1.00 40.74	В
	MOTA	1065		THR	152	15.950	10.748	36.860	1.00 42.40	В
	MOTA	1066	CB	THR	152	16.587	9.674	37.772	1.00 42.88	В
	ATOM	1067	OG1	THR	152	16.143	8.375	37.365	1.00 46.42	В
55	ATOM	1068	CG2		152	16.182	9.891	39.221	1.00 43.02	В
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	ATOM	1069	С	THR	152	16.537	12.108	37.216	1.00 42.92	В
	MOTA	1070	0	THR	152	17.753	12.303	37.176	1.00 45.15	В
	ATOM	1071		GLU	153	15.657	13.050	37.539	1.00 41.16	В
~	MOTA	1072	CA	GLU	153	16.083	14.390	37.910	1.00 39.15	В
60	MOTA	1073	CB	GLU	153	14.902	15.350	37.865	1.00 41.46	В
	MOTA	1074		GLU	153	15.290	16.742	37.456	1.00 46.88	В
	ATOM	1075		GLU	153	15.645	16.826	35.983	1.00 50.26	В
	MOTA	1076	OE1	GLU	153	16.309	17.808	35.591	1.00 54.28	В
	MOTA	1077	OE2		153	15.256	15.920	35.216	1.00 50.49	В
65										
0.5	ATOM	1078		GLU	153	16.601	14.273	39.336	1.00 35.77	В
	MOTA	1079	0	GLU	153	16.024	13.550	40.143	1.00 34.39	В
	ATOM	1080		PHE	154	17.676	14.986	39.649	1.00 32.19	В
	MOTA	1081		PHE	154	18.247	14.903	40.985	1.00 29.64	В
	MOTA	1082	CB	PHE	154	19.221	13.731	41.036	1.00 26.07	В
70	MOTA	1083		PHE	154	20.478	13.959	40.244	1.00 22.24	В
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	MOTA	1084	CD1		154	21.634	14.413	40.870	1.00 19.12	В
	MOTA	1085	CD2	PHE	154	20.502	13.725	38.873	1.00 19.79	В
	ATOM	1086	CEL		154	22.804	14.627	40.140	1.00 20.17	В
	ATOM	1000			123	22.004	24.02/	-0.110	1.00 20.17	В

	MOTA	1087	CE2	PHE	154	21.665	13.938	38.132	1.00 19.68	В
	MOTA	1088	CZ	PHE	154	22.819	14.388	38.768	1.00 18.22	В
	MOTA	1089	c	PHE	154	18.983	16.153	41.462	1.00 28.59	В
	MOTA	1090	ō	PHE	154					
5	ATOM		N			19.343	17.025	40.687	1.00 28.03	В
J		1091		SER	155	19.219	16.194	42.765	1.00 28.62	В
	MOTA	1092	ÇA	SER	155	19.940	17.286	43.398	1.00 29.65	В
	MOTA	1093	CB	SER	155	18.958	18.297	44.007	1.00 29.30	В
	MOTA	1094	OG	SER	155	18.373	17.825	45.210	1.00 30.25	В
10	MOTA	1095	С	SER	155	20.812	16.670	44.495	1.00.29.32	B
10	MOTA	1096	0	SER	155	20.364	15.799	45.236	1.00 28.78	В
	MOTA	1097	N	VAL	156	22.057	17.117	44.601	1.00 28.25	В
	ATOM	1098	CA	VAL	156	22.945	16.571	45.622	1.00 27.65	В
	MOTA	1099	CB	VAL	156	24.266	16.059	45.002	1.00 27.82	В
	ATOM	1100	CG1	VAL	156	25.067	15.296	46.051	1.00 26.25	В
15	MOTA	1101	CG2	VAL	156	23.970	15.178	43.793	1.00 26.92	В
	MOTA	1102	С	VAL	156	23.293	17.600	46.697	1.00 28.00	B
	ATOM	1103	ō	VAL	156	23.691	18.705	46.386	1.00 27.61	В
	ATOM	1104	N	LYS	157	23.135	17.210	47.961	1.00 28.26	В
	ATOM	1105	CA	LYS	157	23.455	18.066	49.107	1.00 29.25	
20	ATOM	1106	CB	LYS	157					В
20						22.188	18.423	49.897	1.00 30.98	В
	MOTA	1107	CG	LYS	157	21.322	19.485	49.261	1.00 34.09	В
	MOTA	1108	CD	LYS	157	20.065	19.741	50.080	1.00 37.95	В
	ATOM	1109	CE	LYS	157	19.399	21.060	49.665	1.00 41.02	В
25	MOTA	1110	NZ	LYS	157	20.186	22.277	50.077	1.00 41.43	В
23	MOTA	1111	C	LYS	157	24.426	17.349	50.047	1.00 28.34	В
	ATOM	1112	0	LYS	157	24.195	16.217	50.413	1.00 28.14	В
	MOTA	1113	N	VAL	158	25.510	18.016	50.433	1.00 27.07	В
	MOTA	1114	CA	VAL	158	26.480	17.412	51.342	1.00 27.48	В
20	MOTA	1115	CB	VAL	158	27.883	17.280	50.694	1.00 26.91	В
30	MOTA	1116		VAL	158	27.811	16.356	49.489	1.00 27.77	В
	MOTA	1117	CG2		158	28.415	18.648	50.301	1.00 27.25	В
	ATOM	1118	С	VAL	158	26.629	18.183	52.651	1.00 28.66	. B
	MOTA	1119	0	VAL	158	26.444	19.393	52.705	1.00 27.69	В
25	MOTA	1120	N	SER	159	26.973	17.460	53.708	1.00 28.98	В
35	MOTA	1121	CA	SER	159	27.155	18.058	55.013	1.00 30.95	B
	ATOM	1122	CB	SER	159	25.869	17.953	55.823	1.00 32.26	В
	ATOM	1123	0G	SER	159	24.817	18.602	55.132	1.00 38.42	В
	MOTA	1124	С	SER	159	28.289	17.362	55.736	1.00 30.96	В
	ATOM	1125	0	SER	159	28.388	16.146	55.722	1.00 34.27	В
40	MOTA	1126	N	LEU	160	29.158	18.143	56.357	1.00 29.31	В
	ATOM	1127	CA	LEU	160	30.280	17.577	57.064	1.00 27.33	В
	MOTA	1128	СВ	LEU	160	31.582	18.130	56.499	1.00 27.18	В
	MOTA	1129	CG	LEU	160	32.856	17.456	56.991	1.00 28.13	В
	MOTA	1130		LEU	160	32.751	15.954	56.790	1.00 29.56	В
45	MOTA	1131		LEU	160	34.044	18.019	56.237	1.00 28.17	B
	MOTA	1132	C	LEU	160	30.167	17.884	58.552	1.00 28.09	В
	ATOM	1133	ō	LEU	160	30.607	18.943	59.026	1.00 26.39	В
	ATOM	1134	N	LEU	161	29.558	16.949	59.276	1.00 25.48	В
	MOTA	1135	CA	LEU	161	29.371	17.075	60.710	1.00 23.19	B
50	ATOM	1136	CB	LEU	161	27.982	16.567	61.101	1.00 21.33	В
	ATOM	1137	CG	LEU	161	27.694	16.395	62.594	1.00 19.50	В
	MOTA	1138		LEU	161	27.772	17.736	63.288	1.00 19.94	В
	ATOM	1139		LEU	161	26.314	15.775	62.782	1.00 17.88	В
	ATOM	1140	c	LEU	161	30.452	16.264	61.415	1.00 23.39	В
55	MOTA	1141	Ö	LEU	161	30.641	15.094	61.129		
	ATOM	1142	N	GLU	162	31.165			1.00 25.56 1.00 22.32	B
	ATOM	1143	CA	GLU		32.232	16.899	62.336		В
					162		16.237	63.065	1.00 19.98	В
	MOTA	1144	CB	GLU	162	33.574	16.839	62.650	1.00 17.28	В
60	MOTA	1145	CG	GLU	162	33.762	16.859	61.137	1.00 15.11	В
UU	MOTA	1146	CD	GLU	162	35.212	16.937	60.737	1.00 15.23	В
	MOTA	1147		GLU	162	36.063	17.134	61.621	1.00 15.82	В
	ATOM	1148		GLU	162	35.513	16.813	59.539	1.00 17.71	В
	ATOM	1149	C	GLU	162	32.031	16.344	64.573	1.00 19.72	В
65	MOTA	1150	0	GLU	162	31.468	17.299	65.059	1.00 20.94	В
65	ATOM	1151	N	ILE	163	32.503	15.348	65.312	1.00 18.63	В
	MOTA	1152	CA	ILE	163	32.346	15.350	66.756	1.00 18.63	В
	MOTA	1153	CB	ILE	163	31.544	14.120	67.223	1.00 19.02	В
	MOTA	1154		ILE	163	31.324	14.178	68.742	1.00 16.34	В
3 0	MOTA	1155		ILE	163	30.210	14.072	66.466	1.00 20.01	В
70	MOTA	1156	CD1	ILE	163	29.479	12.746	66.563	1.00 22.19	В
	MOTA	1157	С	ILE	163	33.694	15.353	67.467	1.00 20.32	В
	ATOM	1158	0	ILE	163	34.616	14.672	67.050	1.00 21.59	В
	MOTA	1159	N	TYR	164	33.799	16.131	68.542	1.00 20.27	В
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						25 424		60.310		
•	MOTA	1160	CA	TYR	164 164	35.031 35.964	16.206 17.271	69.312 68.709	1.00 19.81	B B
	ATOM ATOM	1161 1162	CB	TYR TYR	164	37.269	17.434	69.451	1.00 17.18	В
	MOTA	1163		TYR	164	37.334	18.191	70.622	1.00 16.03	В
5	ATOM	1164		TYR	164	38.506	18.253	71.372	1.00 16.71	В
	MOTA	1165	CD2	TYR	164	38.416	16.756	69.042	1.00 18.67	В
	ATOM .	1166	CE2	TYR	164	39.594	16.812	69.789	1.00 16.74	В
	MOTA	1167	CZ	TYR	164	39.627	17.557	70.954	1.00 14.83	В
10	MOTA	1168	он	TYR	164	40.758	17.569	71.726	1.00 14.97	В
10	MOTA	1169	Ç	TYR	164	34.685	16.520 17.468	70.761 71.044	1.00 21.32	B B
	atom Atom	1170 1171	O N	TYR ASN	164 165	33.971 35.185	15.694	71.672	1.00 22.71	В
	MOTA	1172	CA	ASN	165	34.926	15.860	73.092	1.00 23.78	В
	ATOM	1173	CB	ASN	165	35.722	17.043	73.636	1.00 27.16	В
15	MOTA	1174	CG	ASN	165	35.729	17.090	75.149	1.00 31.99	. В
	MOTA	1175		ASN	165	36.159	16.150	75.801	1.00 37.27	В
	MOTA	1176		ASN	165	35.249	18.190	75.714	1.00 32.43	В
	MOTA	1177	c	ASN	165	33.431	16.088	73.313	1.00 24.23	B B
20	MOTA MOTA	1178 1179	N O	asn Glu	165 166	33.034 32.615	16.915 15.340	74.130 72.572	1.00 22.37	В
20	MOTA	1180	CA	GLU	166	31.154	15.421	72.641	1.00 22.51	В
	MOTA	1181	CB	GLU	166	30.638	15.047	74.044	1.00 19.36	В
	MOTA	1182	CG	GLU	166	30.620	13.540	74.319	1.00 20.22	В
05	MOTA	1183	CD	GLU	166	29.915	12.746	73.222	1.00 20.01	·B
25	MOTA	1184		GLU	166	28.668	12.648	73.240	1.00 19.99	8
	MOTA	1185		GLU	166	30.618	12.228	72.330 72.223	1.00 16.45 1.00 22.98	B B
	MOTA MOTA	1186 1187	C O	GLU	166 166	30.570 29:553	16.770 17.189	72.725	1.00 22.40	В
	MOTA	1188	N	GLU	167	31.229	17.443	71.288	1.00 25.41	В
30	MOTA	1189	CA	CLU	167	30.739	18.721	70.793	1.00 27.30	В
	ATOM	1190	CB	GLU	167	31.679	19.858	71.191	1.00 29.98	В
	MOTA	1191	CG	GLU	167	31.567	20.295	72.648	1.00 34.85	В
	MOTA	1192	CD	GLU	167	32.384	21.553	72.941	1.00 39.75	В
35	ATOM	1193		GLU	167	33.635	21.487	72.865	1.00 39.56	B B
33	MOTA	.1194 1195	C C	GLU	167 167	31.771 30.637	22.608 18.626	73.237 69.278	1.00 41.26	В
	MOTA	1196	ò	GLU	167	31.495	18.046	68.633	1.00 29.56	В
	ATOM	1197	N	LEU	168	29.574	19.190	68.719	1.00 28.34	В
	MOTA	1198	CA	LEU	168	29.367	19.138	67.280	1.00 28.28	В
40	MOTA	1199	CB	LEU	168	27.865	19.078	66.955	1.00 30.49	В
	MOTA	1200	CG	LEU	168	27.009	17.925	67.512	1.00 30.82	В
	ATOM ATOM	1201		LEU	168 168	27.623 25.892	16.583 18.044	67.142 69.009	1.00 31.07	B B
	ATOM	1202 1203	C	LEU	16B	29.997	20.322	66.563	1.00 26.93	В
45	MOTA	1204	ŏ	LEU	168	29.972	21.442	67.064	1.00 28.48	В
	ATOM	1205	N	PHE	169	30.562	20.069	65.386	1.00 24.01	В
	MOTA	1206	CA	PHE	169	31.191	21.112	64.584	1.00 22.5B	В
	MOTA	1207	CB	PHE	169	32.723	21.073	64.727	1.00 22.71	В
50	MOTA	1208	CG	PHE	169	33.213	21.377	66.118	1.00 21.76	B B
J U	MOTA	1209 1210		PHE	169 169	33.451 33.393	20.354 22.699	67.027 66.534	1.00 21.14	B
	ATOM ATOM	1211		PHE	169	33.861	20.628	68.323	1.00 22.05	В
	MOTA	1212		PHE	169	33.802	22.989	67.830	1.00 21.62	. В
	MOTA	1213	CZ	PHE	169	34.037	21.952	68.729	1.00 24.67	В
55	MOTA	1214	C	PHE	169	30.824	20.950	63.111	1.00 23.10	В
	MOTA	1215	0	PHE	169	30.612	19.836	62.634	1.00 20.06	В
	MOTA	1216	N	ASP	170	30.739	22.079	62.406	1.00 22.96	B B.
	MOTA	1217 1218	CA CB	ASP ASP	170 170	30.416 29.344	22.100 23.148	60.978 60.679	1.00 20.54	В.
60	MOTA MOTA	1219	CG	ASP	170	28.799	23.048	59.257	1.00 21.66	В
•	MOTA	1220		ASP	170	29.554	22.671	58.337	1.00 18.77	В
	ATOM	1221		ASP	170	27.602	23.358	59.065	1.00 23.66	В
	MOTA	1222	С	ASP	170	31.680	22.466	60.211	1.00 22.85	В
45	ATOM	1223	0	ASP	170	32.108	23.621	60.242	1.00 25.36	В
65	ATOM	1224	N	LEU	171	32.280	21.490	59.529	1.00 22.35	В
	MOTA	1225	CA	LEU	171	33.494	21.729	58.764	1.00 22.58	B
	atom atom	1226 1227	CB	LEU	171 171	34.430 35.235	20.533	58.864 60.169	1.00 16.27 1.00 16.39	B B
	MOTA	1228		LEU	171	36.234	21.577	60.274	1.00 14.32	В
70	MOTA	1229		LEU	171	34.304	20.421	61.351	1.00 12.71	В
	MOTA	1230	C	LEU	171	33.257	22.082	57.300	1.00 26.58	В
	MOTA	1231	0	LEU	171	34.167	21.976	56.479	1.00 26.75	В
	MOTA	1232	N	LEU	172	32.038	22.510	56.978	1.00 29.45	В

	MOTA	1233	CA	LEU	172	31.706	22.898	55.612	1.00 34.57	В
	ATOM	1234	СВ	LEU	172	30.742	21.892	54.975	1.00 33.36	В.
	MOTA	1235	CG	LEU	172	31.387	20.715	54.244	1.00 31.35	В
•	MOTA	1236	CD1		172	30.316	19.992	53.459	1.00 32.85 1.00 32.08	B B
5	ATOM	1237	CD2		172 172	32.473 31.107	21.201 24.297	53.302 55.531	1.00 32.00	В
	MOTA	1238	0	LEU	172	30.961	24.257	54.457	1.00 39.59	В
	MOTA MOTA	1239 1240	N	ASN	173	30.766	24.865	56.679	1.00 41.36	В
	MOTA	1241	CA	ASN	173	30.201	26.205	56.714	1.00 45.99	В
10	ATOM	1242	СВ	ASN	173	29.401	26.405	58.003	1.00 47.65	В
- •	ATOM	1243	CG	ASN	173	28.670	27.735	58.038	1.00 50.77	В
	MOTA	1244	OD1	ASN	173	28.005	28.060	59.014	1.00 51.85	В
	MOTA	1245	ND2	ASN	173	28.792	28.508	56.964	1.00 51.20	В
	MOTA	1246	С	asn	173	31.346	27.214	56.643	1.00 48.84	В
15	MOTA	1247	0	ASN	173	32.070	27.403	57.606	1.00 48.46	В
	MOTA	1248	N	PRO	174	31.521	27.872	55.484	1.00 52.47	B B
	MOTA	1249	CD	PRO	174	30.710	27.738	54.258 55.289	1.00 53.23 1.00 55.00	В
	MOTA	1250	CA	PRO	174 174	32.587 32.542	28.862 29.116	53.786	1.00 53.00	В
20	MOTA MOTA	1251 1252	CB	PRO PRO	174	31.089	28.983	53.482	1.00 52.93	В
20	ATOM	1253	c	PRO	174	32.396	30.141	56.095	1.00 58.07	В
	MOTA	1254	ŏ	PRO	174	33.329	30.921	56.263	1.00 58.84	В
	MOTA	1255	N	SER	175	31.183	30.343	56.596	1.00 60.39	B
	MOTA	1256	CA	SER	175	30.861	31.534	57.372	1.00 62.65	В
25	MOTA	1257	CB	SER	175	29.343	31.666	57.498	1.00 63.30	В
	MOTA	1258	OG	SER	175	28.723	31.545	56.230	1.00 65.14	В
	MOTA	1259	С	SER	175	31.500	31.535	58.759	1.00 63.89	В
	MOTA	1260	0	SER	175	32.365	32.358	59.051	1.00 65.71	В
20	ATOM	1261	N	SER	176	31.066	30.608	59.608	1.00 64.41 1.00 64.51	B B
30	MOTA		CA	SER	176	31.581	30.506	60.969 61.844	1.00 64.33	В
	MOTA	1263	CB OG	SER	176 176	30.597 30.446	29.725 28.396	61.378	1.00 64.08	В
	MOTA MOTA	1264 1265	C	SER	176	32.942	29.824	61.012	1.00 64.78	В
	ATOM	1266	ŏ	SER	176	33.474	29.418	59.984	1.00 64.25	В
35	ATOM	1267	N	ASP	- 177	33.500	29.704	62.213	1.00 65.17	ъ.
-	ATOM	1268	CA	ASP	177	34.789	29.051	62.379	1.00 65.62	В
	MOTA	1269	CB	ASP	177	35.782	29.964	63.106	1.00 66.73	В
	ATOM	1270	CG	ASP	177	35.449	30.137	64.576	1.00 68.48	В
40	ATOM	1271	OD1	ASP	177	36.388	30.344	65.377	1.00 67.76	В
40	ATOM	1272	OD2	ASP	177	34.251	30.069	64.929	1.00 69.81	В
	MOTA	1273	C	ASP	177	34.615	27.757	63.166 63.445	1.00 64.60 1.00 64.22	B B
	ATOM	1274 1275	O N	ASP VAL	177 178	33.498 35.737	27.335 27.146	63.529	1.00 63.40	В
	ATOM ATOM	1276	CA	VAL	178	35.735	25.890	64.264	1.00 62.69	В
45	MOTA	1277	CB	VAL	178	37.046	25.116	64.016	1.00 62.85	. В
	MOTA	1278		VAL	178	37.190	24.809	62.536	1.00 61.71	В
	MOTA	1279		VAL	178	38.231	25.934	64.510	1.00 62.99	В
	ATOM	1280	С	VAL	178	35.552	26.050	65.770	1.00 61.94	В
	MOTA	1281	0	VAL	178	35.792	25.122	66.524	1.00 62.60	В
50	MOTA	1282	N	SER	179	35.124	27.227	66.208	1.00 61.07	В
	MOTA	1283	CA	SER	179	34.922	27.447	67.632	1.00 59.46 1.00 59.42	B B
	MOTA	1284	CB	SER	179	35.629	28.731	68.080 67.507	1.00 59.42	B
	MOTA	1285 1286	OG C	SER	179 179	35.030 33.437	29.877 27.517	67.977	1.00 58.68	В
55	MOTA MOTA	1287	o	SER	179	33.067	27.489	69.144	1.00 59.17	В
55	ATOM	1288	N	GLU	180	32.591	27.605	66.955	1.00 56.65	В
	ATOM	1289	CA	GLU	180	31.145	27.671	67.161	1.00 55.22	В
	MOTA	1290	CB	GLU	180	30.507	28.607	66.129	1.00 56.66	В
	MOTA	1291	CG	GLU	180	30.550	30.079	66.535	1.00 59.12	В
60	MOTA	1292	CD	GLU	180	30.230	31.032	65.392	1.00 60.03	В
	MOTA	1293	OE1	GLU	180	31.066	31.163	64.474	1.00 60.45	В
	MOTA	1294	OE2	GLU	180	29.143	31.650	65.411	1.00 61.47	В
	ATOM	1295	С	GLU	180	30.498	26.293	67.080	1.00 52.95	В
45	MOTA	1296	0	GLU	180	30.207	25.803	66.004	1.00 52.86	. B
65	MOTA	1297	N	ARG	181	30.285	25.679	68.239	1.00 51.12	9 B
	MOTA	1298	CA	ARG	181	29.675	24.360	68.315	1.00 48.73	В В
	MOTA	1299	CB	ARG	181	29.835	23.793	69.727 70.836	1.00 51.62 1.00 56.45	В
	MOTA	1300	CG	ARG	181	29.642 28.829	24.816 24.256	72.007	1.00 50.45	В
70	MOTA MOTA	1301 1302	NE NE	ARG ARG	181 181	27.400	24.236	71.702	1.00 64.33	В
70	MOTA	1302	CZ	ARG	181	26.483	23.692	72.560	1.00 65.71	В
	MOTA	1304		ARG	181	26.834	23.324	73.786	1.00 66.05	В
	ATOM	1305		ARG	181	25.209	23.616	72.194	1.00 66.36	В
			-							

	MOTA MOTA	1306 1307	С 0	ARG ARG	181 181	28.196 27.556	24.403 25.438	67.940 68.029	1.00 45.46 1.00 45.33	B B
	ATOM	1308	N	LEU	182	27.661	23.267	67.510	1.00 41.98	В
5	ATOM	1309	CA	LEU	182	26.258	23.193	67.133 65.824	1.00 38.04 1.00 35.02	B B
,	MOTA MOTA	1310 1311	CB CG	LEU	182 182	26.099 26.990	22.419 22.896	64.677	1.00 33.00	В
	ATOM	1312		LEU	182	26.723	22.060	63.450	1.00 31.57	В
	ATOM	1313		LEU	182	26.733	24.372	64.393	1.00 32.49	В
••	MOTA	1314	С	LEU	182	25.456	22.524	68.236	1.00 38.00	В
10	ATOM	1315	0	LEU	182	26.017	21.845	69.096	1:00 37.75	В
	ATOM	1316	N	GLN	183	24.140 23.239	22.723	68.206 69.200	1.00 37.43	B B
	MOTA MOTA	1317 1318	CA	GLN	183 183	23.239 · 22.269	22.148 23.210	69.724	1.00 38.87	В
	ATOM	1319	CG	GLN	183	22.925	24.543	70.024	1.00 43.04	В
15	ATOM	1320	CD	GLN	183	21.969	25.536	70.653	1.00 45.13	B
	MOTA	1321		GLN	183	21.663	25.448	71.832	1.00 45.23	В
	MOTA	1322	NE2	GLN	183	21.493	26.492	69.856	1.00 46.40	В
	MOTA MOTA	1323 1324	C	GLN	183 183	22.455 22.097	21.018 21.073	68.567 67.397	1.00 35.80	B B
20	ATOM	1325	N	MET	184	22.165	20.005	69.367	1.00 36.43	В
	MOTA	1326	CA	MET	184	21.450	18.840	68.877	1.00 37.65	В
	ATOM	1327	CB	MET	184	22.322	17.610	69.118	1.00 38.53	₿.
	ATOM	1328	CG	MET	184	22.033	16.445	68.221	1.00 41.45	В
25	ATOM	1329	SD	MET	184	23.141	15.085	68.586	1.00 42.59	B B
23	MOTA MOTA	1330 1331	CE	MET	184 184	22.590 20.111	14.660 18.692	70.190 69.590	1.00 40.16 1.00 37.82	В
	ATOM	1332	ŏ	MET	184	20.021	18.909	70.790	1.00 37.22	В
	ATOM	1333	N	PHE	185	19:070	18.328	68.844	1.00 39.01	В
20	MOTA	1334	CA	PHE	185	17.741	18.148	69.432	1.00 41.26	В
30	ATOM	1335	CB	PHE	185	16.851	19.377	69.160	1.00 40.10	В
	MOTA MOTA	1336 1337	CC	PHE	185 185	17.499 18.249	20.697 21.377	69.494 68.544	1.00 38.50 1.00 36.52	B B
	ATOM	1338		PHE	185	17.376	21.248	70.770	1.00 38.29	В
	MOTA	1339		PHE	185	18.869	22.586	68.851	1.00 37.06	В
35	MOTA	-1340		PHE	185	17.994	22.459	71.089	1.00 37.60	В
	MOTA	1341	cz	PHE	185	18.743	23.128	70.128	1.00 37.41	В
	ATOM ATOM	1342 1343	C O	PHE	185 185	17.034 17.221	16.903 16.532	68.887 67.734	1.00 43.21 1.00 41.62	B B
	ATOM	1343	N	ASP	186	16.223	16.259	69.724	1.00 46.68	В
40	ATOM	1345	CA	ASP	186	15.482	15.078	69.286	1.00 51.00	В
	MOTA	1346	CB	ASP	186	14.722	14.437	70.449	1.00 52.32	В
	MOTA	1347	CG	ASP	186	15.642	13.912	71.530	1.00 54.63	В
	MOTA	1348		ASP	186	16.575	13.150	71.202	1.00 55.59	В
45	MOTA MOTA	1349 1350	C C	ASP	186 186	15.428 14.481	14.262 15.539	72.712 68.241	1.00 56.98 1.00 52.48	B B
	MOTA	1351	ŏ	ASP	186	13.777	16.510	68.443	1.00 52.99	В
	MOTA	1352	N	ASP	187	14.425	14.841	67.118	1.00 55.70	В
	ATOM	1353	CA	ASP	187	13.500	15.214	66.061	1.00 59.24	В
50	MOTA	1354	CB	ASP	187	13.845	14.469	64.772	1.00 58.33	В
50	MOTA	1355 1356	CG	ASP	187 187	13.015 13.345	14.929 14.546	63.601 62.459	1.00 58.32 1.00 59.29	B B
	MOTA	1357		ASP	187	12.035	15.672	63.822	1.00 58.82	В
	MOTA	1358	С	ASP	187	12.064	14.905	66.473	1.00 61.85	В
55	MOTA	1359	0	ASP	187	11.690	13.750	66.626	1.00 62.59	В
55	MOTA	1360	N	PRO	188	11.241	15.950	66.662	1.00 64.18	В
	ATOM	1361 1362	CD	PRO PRO	188 188	11.573 9.840	17.374 15.794	66.493 67.061	1.00 64.61	B B
	MOTA	1363	CB	PRO	188	9.287	17.207	66.923	1.00 65.95	В
	ATOM	1364	CG	PRO	188	10.472	18.048	67.271	1.00 65.81	В
60 ·	MOTA	1365	С	PRO	188	9.094	14.793	66.189	1.00 68.16	В
	MOTA	1366	0	PRO	188	8.316		66.687	1.00 67.45	В
	MOTA	1367 1368	N CA	ARG ARG	189	9.345	14.854	64.886	1.00 70.27	B B
	MOTA	1369	CB	ARG	189 189	8.702 9.278	13.949 14.170	63.944 62.547	1.00 73.94	В
65	ATOM	1370	CG	ARG	189	8.869	15.498	61.926	1.00 75.92	В
	MOTA	1371	CD	ARG	189	9.507	15.693	60.558	1.00 77.54	В
	HOTA	1372	NE	ARG	189	10.797	16.373	60.644	1.00 78.29	В
	MOTA	1373	CZ	ARG	189	10.940	17.686	60.804	1.00 78.57	8
70	MOTA MOTA	1374 1375		ARG ARG	189 189	9.870 12.153	18.466 18.218	60.894 60.873	1.00 78.77 1.00 78.05	B B
, 0	ATOM	1376	C	ARG	189	8.869	12.491	64.363	1.00 75.30	В
	ATOM	1377	ō	ARG	189	7.896	11.815	64.683	1.00 75.56	В
	ATOM	1378	N	ASN	190	10.112	12.019	64.370	1.00 77.42	В

	MOTA	1379	CA	ASN	190	10.417	10.640	64.748	1.00 78.69	В
	MOTA	1380	CB	ASN	190	10.760	9.829	63.494	1.00 78.94	В
	ATOM	1381	CG	ASN	190	11.569	10.629	62.483	1.00 78.61	В
									1.00 78.52	В
5	MOTA	1382		ASN	190	12.745	10.905	62.689		
J	MOTA	1383		asn	190	10.926	11.011	61.383	1.00 78.16	В
	MOTA	1384	C	ASN	190	11.571	10.575	65.749	1.00 79.40	В
	MOTA	1385	0	ASN	190	12.706	10.875	65.408	1.00 79.98	В
	MOTA	1386	N	LYS	191	11.265	10.182	66.986	1.00 79.97	В
	ATOM	1387	CA	LYS	191	12.267		68.051	1.00 79.77	В
10	ATOM	1388	CB	LYS	191	11.616	9.561	69.336	1.00 81.11	В
10					191	10.794	10.600	70.090	1.00 82.60	В
	MOTA	1389	CG	LYS						
	MOTA	1390	CD	LYS	191	11.695	11.630	70.758	1.00 83.37	В
	MOTA	1391	CE	LYS	191	10.887	12.716	71.450	1.00 84.12	В
	ATOM	1392	NZ	LYS	191	10.109	13.539	70.478	1.00 84.72	В
15	ATOM	1393	Ç	LYS	191	13.478	9.216	67.695	1.00 78.46	В
	ATOM	1394	0	LYS	191	14.462	9.173	68.434	1.00 77.59	В
	ATOM	1395	N	ARG	192	13.398	8.525	66.563	1.00 76.93	В
	ATOM	1396	CA	ARG	192	14.489	7.675	66.106	1.00 75.17	В
	ATOM	1397	СВ	ARG	192	13.975	6.667	65.078	1.00 77.95	В
20								64.573	1.00 80.81	В
20	MOTA	1398	CG	ARG	192	15.041	5.708			
	ATOM	1399	CD	ARG	192	14.801	5.305	63.122	1.00 83.98	В
	ATOM	1400	NE	ARG	192	14.928	6.434	62.198	1.00 86.03	В
	MOTA	1401	CZ	ARG	192	13.946	7.277	61.884	1.00 86.70	В
	ATOM	1402	NH1	ARG	192	12.737	7.133	62.415	1.00 86.57	В
25	MOTA	1403	NH2	ARG	192	14.175	8.267	61.033	1.00 87.03	В
_ •	ATOM	1404	C	ARG	192	15.565	8.545	65.463	1.00 72.66	В
	ATOM	1405		ARG	192	16.699	8.112	65.272	1.00 72.31	В
				GLY	193	15.195	9.781	65.136	1.00 69.32	В
	MOTA	1406	N							В
20	ATOM	1407	CA	GLY	193	16.132	10.695	64.507	1.00 63.90	
30	MOTA	1408	С	GLY	193	16.538	11.863	65.382	1.00 59.50	В
	MOTA	1409	0	GLY	193	16.132	11.961	66.531	1.00 59.54	В
	MOTA	1410	N	VAL	194	17.346	12.757	64.824	1.00 55.13	В
	ATOM	1411	CA	VAL	194	17.812	13.918	65.562	1.00 50.91	В
	MOTA	1412	CB	VAL	194	19.114	13.606	66.309	1.00 50.28	В
35	ATOM	1413		VAL	194	20.226	13.319	65.318	1.00 49.18	В
	MOTA	1414		VAL	194	19.476	14.760	67.207	1.00 48.67	В
					194	18.055	15.098	64.629	1.00 49.13	В
	MOTA	1415	C	VAL					1.00 49.22	
	MOTA	1416	0	VAL	194	18.379	14.918	63.461		В
40	ATOM	1417	N	ILE	195	17.906	16.308	65.160	1.00 46.55	В
40	MOTA	1418	CA	ILE	195	18.106	17.514	64.372	1.00 42.49	В
	ATOM	1419	CB	ILE	195	16.846	18.405	64.396	1.00 43.57	В
	MOTA	1420	CG2	ILE	195	17.076	19.653	63.561	1.00 44.86	В
	MOTA	1421	CG1	ILE	195	15.647	17.639	63.837	1.00 44.25	В
	ATOM	1422		ILE	195	15.828	17.184	62.393	1.00 45.64	В
45	ATOM	1423	c	ILE	195	19.291	18.349	64.856	1.00 39.72	В
73			ō			19.379	18.691	66.030	1.00 38.69	В
	MOTA	1424		ILE	195					В
	ATOM	1425	N	ILE	196	20.197	18.672	63.936	1.00 37.40	
	MOTA	1426	CA	ILE	196	21.365	19.483	64.255	1.00 35.21	В
50	MOTA	1427	CB	ILE	196	22.654	18.960	63.561	1.00 34.42	В
50	ATOM	1428	CG2	ILE	196	23.821	19.880	63.881	1.00 33.62	В
	MOTA	1429	CG1	ILE	196	23.010	17.552	64.057	1.00 33.50	В
	ATOM	1430	CD1	ILE	196	22.222	16.445	63.416	1.00 31.23	В
	ATOM	1431	С	ILE	196	21.113	20.920	63.806	1.00 35.34	В
	ATOM	1432	ō	ILE	196	21.108	21.218	62.619	1.00 33.58	В
55	ATOM	1433	N	LYS	197	20.912	21.806	64.777	1.00 36.02	В
33									1.00 36.95	В
	ATOM	1434	CA	LYS	197	20.639	23.209	64.494		
•	Atom	1435	CB	LYS	197	20.101	23.909	65.744	1.00 37.83	В
	MOTA	1436	CG	LYS	197	19.736	25.370	65.519	1.00 42.01	В
	MOTA	1437	CD	LYS	197	19.391	26.055	66.829	1.00 45.50	В
60	MOTA	1438	CE	LYS	197	19.039	27.518	66.628	1.00 46.65	В
	ATOM	1439	NZ	LYS	197	18.686	28.161	67.932	1.00 47.32	В
	MOTA	1440	c	LYS	197	21.857	23.968	63.983	1.00 36.01	В
									1.00 34.47	8
	ATOM	1441	0	LYS	197	22.887	24.025	64.646		
65	MOTA	1442	N	GLY	198	21.722	24.547	62.793	1.00 35.82	В
65	ATOM	1443	CA	GLY	198	22.809	25.316	62.212	1.00 37.33	В
	MOTA	1444	С	GLY	198	23.715	24.583	61.240	1.00 38.13	В
	MOTA	1445	0	GLY	198	24.580	25.198	60.615	1.00 39.69	В
	ATOM	1446	N	LEU	199	23.530	23.275	61.098	1.00 37.34	В
	ATOM	1447	CA	LEU	199	24.376	22.512	60.190	1.00 36.62	В
70	ATOM	1448	СВ	LEU	199	24.218	21.006	60.444	1.00 34.70	В
. •	ATOM	1449	CG	LEU	199	25.067	20.058	59.588	1.00 33.44	В
										В
	ATOM	1450		LEU	199	26.553	20.355	59.755	1.00 31.11	
	ATOM	1451	CD2	LEU	199	24.767	18.634	59.994	1.00 32.49	В

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	MOTA	1452	С	LEU	199	24.066	22,838	58.729	1.00 36.33	В
	MOTA	1453	0	LEU	199	22.971	22.550	58.228	1.00 35.86	В
	ATOM	1454	N	GLU	200	25.040	23.441	58.053	1.00 35.51	В
	ATOM	1455	CA	GLU	200	24.896	23.815	56.653	1.00 37.46	В
5	ATOM	1456	CB	GLU	200	26.037	24.746	56.234	1.00 40.69	В
-		1457	CG	GLU	200	26.005	26.135	56.868	1.00 49.20	В
	MOTA									В
	MOTA	1458	CD	GLU	200	24.757	26.925	56.502	1.00 51.96	
	MOTA	1459		GLU	200	23.659	26.576	56.990	1.00 54.11	В
	MOTA	1460	0E2	GLU	200	24.873	27.896	55.722	1.00 54.04	В
10	ATOM	1461	С	GLU	200	24.874	22.612	55.717	1.00 36.14	В
	MOTA	1462	.0	GLU	200	25.434	21.564	56.015	1.00 35.01	B
	ATOM	1463	N	GLU	201	24.217	22.787	54.575	1.00 35.47	В
								53.559		В
	ATOM	1464	CA	GLU	201	24.124	21.752		1.00 34.36	
1.0	MOTA	1465	CB	GLU	201	22.709	21.189	53.483	1.00 34.40	В
15	ATOM	1466	CG	GLU	201	22.207	20.582	54.773	1.00 34.93	В
	MOTA	1467	CD	GLU	201	20.816	19.998	54.626	1.00 36.86	В
•	ATOM	1468	OE1	GLU	201	20.137	19.825	55.665	1.00 37.44	В
	MOTA	1469		GLU	201	20.408	19.710	53.476	1.00 36.10	В
		1470	C	GLU	201	24.479	22.393	52.226	1.00 34.09	В
20	MOTA									В
20	MOTA	1471	0	GLU	201	23.681	23.115	51.657	1.00 33.70	
	MOTA	1472	N	ILE	202	25.687	22.127	51.740	1.00 33.17	В
	MOTA	1473	CA	ILE	202	26.130	22.689	50.472	1.00 32.42	₿.
	ATOM	1474	CB	ILE	202	27.679	22.715	50.357	1.00 33.25	В
	MOTA	1475	CG2	ILE	202	28.087	23.275	49.002	1.00 31.31	В
25	ATOM	1476		ILE	202	28.286	23.582	51.465	1.00 33.81	В
23				ILE	202	28.222	22.967	52.849	1.00 36.54	В
	MOTA	1477								
	MOTA	1478	Ç	ILE	202	25.572	21.888	49.305	1.00 31.15	В
	MOTA	1479	0	ILE	202	25:703	20.678	49.257	1.00 33.14	В
	MOTA	1480	N	THR	203	24.948	22.583	48.361	1.00 29.99	В
30	MOTA	1481	CA	THR	203	24.371	21.944	47.185	1.00 27.86	В
	MOTA	1482	CB	THR	203	23.228	22.804	46.572	1.00 27.52	В
	ATOM	1483		THR	203	22.157	22.925	47.516	1.00 27.78	В
				THR	203	22.701	22.174	45.284	1.00 26.79	В
	MOTA	1484								
25.	MOTA	1485	С	THR	203	25.448	21.741	46.130	1.00 27.11	В
35 ·	MOTA	.1486	0	THR	203	26.217	22.637	45.853	1.00 26.94	В
	MOTA	1487	N	VAL	204	25.500	20.541	45.560	1.00 27.55	В
	MOTA	1488	CA	VAL	204	26.467	20.222	44.517	1.00 27.42	В
	MOTA	1489	CB	VAL	204	27.136	18.859	44.781	1.00 25.01	В
	ATOM	1490		VAL	204	28.393	18.718	43.941	1.00 23.11	В
40					204	27.468	18.729	46.250	1.00 23.76	В
70	MOTA	1491		VAL						
	MOTA	1492	C	VAL	204	25.677	20.178	43.207	1.00 29.81	В
	ATOM	1493	0	VAL	204	24.887	19.261	42.983	1.00 30.56	В
	MOTA	1494	N	HIS	205	25.891	21.188	42.364	1.00 30.97	В
	MOTA	1495	ÇA	HIS	205	25.197	21.318	41.079	1.00 33.24	В
45	ATOM	1496	CB	HIS	205	25.199	22.792	40.649	1.00 33.42	В
	ATOM	1497	CG	HIS	205	24.641	23.716	41.687	1.00 34.00	В
							24.333	42.739	1.00 33.05	В
	MOTA	1498		HIS	205	25.233				
	MOTA	1499		HIS	205	23.297	24.019	41.771	1.00 33.23	В
~~	MOTA	1500	CEI	HIS	205	23.086	24.777	42.832	1.00 33.03	В
50	ATOM	1501	NE2	HIS	205	24.244	24.981	43.437	1.00 32.48	В
•	MOTA	1502	С	HIS	205	25.790	20.450	39.969	1.00 33.72	В
	MOTA	1503	0	HIS	205	25.084	20.022	39.061	1.00 32.22	В
	ATOM	1504	N	ASN	206	27.094	20.201	40.048	1.00 35.23	В
		1505	CA	ASN	206	27.779	19.381	39.055	1.00 36.89	В
55	ATOM									
22	ATOH	1506	CB	ASN	.:206	28.178	20.229	37.837	1.00 37.95	В
	ATOM	1507	€G	asn	206	28.999	21.455	38.213	1.00 4134	В
	ATOM	1508	OD1	ASN	206	30.130	21.339	38.697	1.00 43.10	В
	ATOM	1509	ND2	ASN	206	28.428	22.641	37.993	1.00 38.53	В
	MOTA	1510	С	ASN	206	29.007	18.712	39.666	1.00 36.43	В
60 ·	MOTA	1511	ō	ASN	206	29.233	18.805	40.864	1.00 36.95	В
00							10.005			В
	MOTA		N	LYS	207		18.029		1.00 36.70	
	ATOM	1513	CA	LYS	207	30.983	17.338	39.297	1.00 37.65	В
	MOTA	1514	CB	LYS	207	31.357	16.232	38.314	1.00 38.65	В
	MOTA	1515	CG	LYS	207	31.892	16.726	36.977	1.00 41.42	В
65	MOTA	1516	CD	LYS	207	31.938	15.585	35.966	1.00 45.62	В
	ATOM	1517	CE	LYS	207	32.889	15.877	34.814	1.00 47.44	B
	ATOM								1.00 47.44	
		1518	NZ	LYS	207	34.314	15.937	35.262		8
	MOTA	1519	Ç	LYS	207	32.155	18.298	39.464	1.00 38.02	В
70	MOTA	1520	0	LYS	207	32.990	18.121	40.340	1.00 38.46	В
70	MOTA	1521	N	ASP	208	32.199	19.320	38.618	1.00 38.91	В
	MOTA	1522	CA	ASP	208	33.264	20.313	38.667	1.00 40.47	B
	MOTA	1523	CB	ASP	208	33.316	21.061	37.338	1.00 42.51	В
	MOTA	1524	CG	ASP						В
	ATON	1324	CO	nor	208	33.664	20.156	36.192	1.00 44.26	ь

	ATOM	1525	OD1	ASP	208	33.297	20.470	35.041	1.00 44.33	В
	ATOM	1526	OD2		208	34.321	19.127	36.451	1.00 46.27	В
					208	33.058	21.300	39.805	1.00 39.34	В
	MOTA	1527	С	ASP				39.780	1.00 40.79	B
~	MOTA	1528	0	ASP	208	33.568	22.405			
5	MOTA	1529	N	GLU	209	32.308	20.893	40.813	1.00 38.81	В
	MOTA	1530	CA	GLU	209	32.050	21.772	41.930	1.00 38.33	₿
	MOTA	1531	CB	GLU	209	30.504	22.260	41.866	1.00 39.47	В
	MOTA	1532	CG	GLU	209	30.278	23.400	42.805	1.00 42.87	В
			CD	GLU	209	28.824	23.836	42.700	1.00 44.43	B
10	MOTA	1533						41.573	1.00 42.49	В
10	MOTA	1534	OE1		209	28.373	24.134			В
	MOTA	1535	OE2		209	28.135	23.885	43.749	1.00 44.53	
	MOTA	1536	С	GLU	209	32.303	21.055	43.247	1.00 37.83	В
	MOTA	1537	0	GLU	209	32.147	21.649	44.316	1.00 38.61	В
	MOTA	1538	N	VAL	210	32.720	19.790	43.171	1.00 35.54	В
15	ATOM	1539	CA	VAL	210	32.954	19.011	44.384	1.00 32.37	В
13		1540	CB	VAL	210	32.679	17.485	44.158	1.00 31.94	В
	MOTA						17.286	43.057	1.00 31.12	В
	ATOM	1541	CG1		210	31.641				В
	ATOM	1542	CG2		210	33.961	16.749	43.842	1.00 30.76	
	MOTA	1543	С	VAL	210	34.342	19.173	44.991	1.00 29.97	В
20	MOTA	1544	0	VAL	210	34.482	19.206	46.207	1.00 29.98	В
	MOTA	1545	N	TYR	211	35.367	19.285	44.154	1.00 27.29	В
	MOTA	1546	CA	TYR	211	36.718	19.408	44.685	1.00 25.19	B
	ATOM	1547	СВ	TYR	211	37.747	19.437	43.549	1.00 24.73	B
				TYR	211	39.177	19.352	44.040	1.00 26.20	В
25	MOTA	1548	CG							B
23	MOTA	1549	CD1		211	39.601	18.278	44.824	1.00 27.98	
	MOTA	1550	CE1	TYR	211	40.903	18.214	45.325	1.00 27.65	В
	MOTA	1551	CD2	TYR	211	40.093	20.360	43.761	1.00 26.06	₿
	ATOM	1552	CE2	TYR	211	41.398	20.308	44.257	1.00 26.72	B
	MOTA	1553	CZ	TYR	211	41.797	19.233	45.041	1.00 29.28	В
30	ATOM	1554	ОН	TYR	211	43.081	19.193	45.556	1.00 27.76	B
50	ATOM	1555	c.	TYR	211	36.864	20.635	45.573	1.00 24.67	В
							20.578	46.615	1.00 24.02	В
	ATOM	1556	0	TYR	211	37.515				
	MOTA	1557	N	GLN	212	36.251	21.742	45.160	1.00 25.05	В
~-	MOTA	1558	CA	GLN	212	36.294	22.982	45.926	1.00 24.24	В
35	MOTA	1559	CB	GLN	212	35.50B	24.082	45.224	1.00 27.89	В
	MOTA	1560	CG	GLN	212	36.375	25.051	44.459	1.00'36.14	В
	MOTA	1561	CD	GLN	212	35.625	26.311	44.048	1.00 40.99	В
	ATOM	1562		GLN	212	34.641	26.248	43.312	1.00 42.51	В
					212	36.090	27.465	44.532	1.00 41.52	В
40	MOTA	1563	NE2							
40	MOTA	1564	С	GLN	212	35.713	22.777	47.305	1.00 22.91	В
	MOTA	1565	0	GLN	212	36.285	23.206	48.299	1.00 23.35	В
	MOTA	1566	N	ILE	213	34.560	22.122	47.362	1.00 22.44	В
	ATOM	1567	CA	ILE	213	33.905	21.876	48.640	1.00 22.31	В
	MOTA	1568	CB	ILE	213	32.595	21.095	48.472	1.00 20.76	В
45	ATOM	1569		ILE	213	31.910	20.947	49.828	1.00 21.01	В
7.5				ILE	213	31.675	21.821	47.492	1.00 20.79	В
	MOTA	1570							1.00 22.47	В
	MOTA	1571		ILE	213	30.457	21.012	47.071		
	MOTA	1572	С	ILE	213	34.816	21.095	49.573	1.00 22.67	В
	ATOM	1573	0	ILE	213	34.863	21.366	50.764	1.00 23.38	В
50	ATOM	1574	N	LEU	214	35.539	20.126	49.020	1.00 24.93	В
	MOTA	1575	CA	LEU	214	36.455	19.307	49.811	1.00 26.22	В
	MOTA	1576	CB	LEU	214	36.965	18.129	48.972	1.00 27.09	В
	MOTA	-1577	CG	LEU	214	36.092	16.868	48.882	1.00 29.34	.B
						34.618	17.235	48.836	1.00 30.24	В
55	MOTA	1578		LEU	214					В
22	MOTA	1579	CD2	LEU	214	36.491	16.059	47.649	1.00 30.55	
	MOTA	1580	С	LEU	214	37.621	20.149	50.314	1.00 26.01	В
	MOTA	1581	0	LEU	214	38.064	19.994	51.444	1.00 26.33	В
	MOTA	1582	N	GLU	215	38.108	21.049	49.464	1.00 25.83	В
	ATOM	1583	CA	GLU	215	39.215	21.930	49.834	1.00 24.69	В
60	ATOM	1584	CB	GLU	215	39.586	22.830	48.655	1.00 23.60	В
00										В
	ATOM	1585	CC	GLU	215	40.814	22.380	47.882	1.00 22.50	
	MOTA	1586	CD	GLU	215	40.907	23.030	46.511	1.00 23.11	В
	MOTA	1587		GLU	215	42.047	23.251	46.040	1.00 20.98	В
	MOTA	1588	OE2	GLU	215	39.839	23.306	45.913	1.00 20.38	В
65	ATOM	1589	С	GLU	215	38.837	22.784	51.040	1.00 23.82	В
	ATOM	1590	ō	GLU	215	39.636	22.960	51.967	1.00 23.91	В
							23.306	51.033	1.00 22.14	В
	MOTA	1591	N	LYS	216	37.617				В
	MOTA	1592	CA	LYS	216	37.152	24.135	52.129	1.00 24.81	
70	MOTA	1593	CB	LYS	216	35.794	24.747	51.781	1.00 28.88	. B
70	ATOM	1594	CG	LYS	216	35.875	25.760	50.637	1.00 35.31	. В
	ATOM	1595	CD	LYS	216	34.492	26.263	50.229	1.00 40.73	В
	ATOM	1596	CE	LYS	216	34.591	27.386	49.208	1.00 42.22	В
	MOTA	1597	NZ	LYS	216	35.405	27.007	48.007	1.00 44.86	В
	WI ON	1331		ت ب ب	2.4.0	33.403	2		2	_

	MOTA	1598	С	LYS	216	37.066	23.327	53.417	1.00 24.49	В
	MOTA	1599	0	LYS	216	37.497	23.790	54.475	1.00 25.43	В
	MOTA	1600	N	GLY	217	36.525	22.117	53.325	1.00 22.80	В
	MOTA	1601	CA	GLY	217	36.427	21.282	54.498	1.00 21.61	В
5	MOTA	1602	C	GLY	217	37.813	21.056	55.063	1.00 21.73	В
-	MOTA	1603	ŏ	GLY	217	38.019	21.154	56.273	1.00 21.45	В
	ATOM	1604	N	ALA	218	38.770	20.770	54.182	1.00 19.63	В
	MOTA	1605	CA	ALA	218	40.146	20.522	54.607	1.00 20.23	В
	ATOM	1606	CB	ALA	218	41.013	20.194	53.402	1.00 20.86	В
10						40.720		55.358	1.00 20.00	В
10	MOTA	1607	C	ALA	218		21.717			B
	MOTA	1608	.0	ALA	218	41.151	21.588	56.500	1.00 21.17	В
	ATOM	1609	N	ALA	219	40.725	22.877	54.706	1.00 19.70	
	MOTA	1610	CA	ALA	219	41.248	24.111	55.299	1.00 18.89	В
15	MOTA	1611	CB	ALA	219	40.928	25.296	54.400	1.00 17.46	В
13	MOTA	1612	С	ALA	219	40.672	24.357	56.675	1.00 18.82	В
	MOTA	1613	0	ALA	219	41.394	24.630	57.621	1.00 19.06	В
	MOTA	1614	N	LYS	220	39.355	24.266	56.778	1.00 19.83	В
	MOTA	1615	CA	LYS	220	38.698	24.501	58.049	1.00 21.65	В
20	MOTA	1616	CB	LYS	220	37.179	24.475	57.867	1.00 22.34	В
20	MOTA	1617	CG	LYS	220	36.416	24.906	59.101	1.00 25.89	В
	MOTA	1618	CD	LYS	220	35.002	25.363	58.759	1.00 28.36	В
	MOTA	1619	CE	LYS	220	34.296	25.886	60.002	1.00 28.81	₿.
	ATOM	1620	NZ	LYS	220	32.888	26.286	59.732	1.00 27.62	В
0.5	MOTA	1621	С	LYS	220	39.145	23.486	59.101	1.00 21.92	-B
25	MOTA	1622	0	LYS	220	39.199	23.807	60.278	1.00 23.01	В
	MOTA	1623	N	ARG	221	39.478	22.268	58.672	1.00 21.66	В
	MOTA	1624	CA	ARG	221	39.934	21.223	59.596	1.00 20.06	В
	MOTA	1625	CB	ARG	221	40:015	19.878	58.882	1.00 22.12	В
	ATOM	1626	CG	ARG	221	38.739	19.076	58.916	1.00 23.91	В
30	ATOM	1627	CD	ARG	221	38.952	17.787	58.173	1.00 26.21	В
	ATOM	1628	NE	ARG	221	37.777	16.929	58.203	1.00 27.96	В
	MOTA	1629	cz	ARG	221	37.620	15.882	57.407	1.00 27.08	В
	MOTA	1630		ARG	221	38.571	15.583	56.529	1.00 25.16	В
	MOTA	1631		ARG	221	36.519	15.145	57.491	1.00 27.49	В
35	ATOM	.1632	С	ARG	221	41.301	21.562	60.167	1.00 18.78	В
	MOTA	1633	ō	ARG	221	41.623	21.206	61.315	1.00 16.42	В
	ATOM	1634	N	THR	222	42.101	22.238	59.350	1.00 15.19	В
	ATOM	1635	CA	THR	222	43.433	22.659	59.741	1.00 15.22	В
	ATOM	1636	CB	THR	222	44.119	23.409	58.593	1.00 16.99	В
40	ATOM	1637		THR	222	44.121	22.573	57.424	1.00 16.46	В
	ATOM	1638		THR	222	45.534	23.796	58.977	1.00 14.73	В
	ATOM	1639	C	THR	222	43.323	23.601	60.928	1.00 16.64	В
	MOTA	1640	ŏ	THR	222	44.046	23.461	61.920	1.00 16.06	В
	MOTA	1641				42.405	24.559	60.828	1.00 16.39	В
45	ATOM		N	THR	223				1.00 17.40	В
13		1642	CA	THR	223	42.202	25.515	61.902		
	MOTA	1643	CB	THR	223	41.160	26.603	61.519	1.00 18.18 1.00 22.16	B B
	MOTA	1644		THR	223	39.839	26.125	61.780		
	MOTA	1645		THR	223	41.268	26.953	60.048	1.00 18.76	В
50	MOTA	1646	c	THR	223	41.708	24.757	63.134	1.00 17.96	В
50	ATOM	1647	0	THR	223	42.078	25.083	64.253	1.00 20.22	В
	MOTA	1648	N	ALA	224	40.875	23.743	62.916	1.00 17.09	В
	MOTA	1649	CA	ALA	224	40.348	22.953	64.027	1.00 17.61	В
	ATOM	1650	CB	ALA	224	39.349	21.902	63.520	1.00 17.42	В
55	ATOM	1651	C	ALA	224	41.503	22.268	64.744	1.00 16.75	В
22	MOTA	1652	0	ALA	224	41.588	22.284	65.979	1.00 13.71	В
	MOTA	1653	N	ALA	225	42.384	21.663	63.950	1.00 16.23	В
	MOTA	1654	CA	ALA	225	43.551	20.980	64.486	1.00 15.92	В
	MOTA	1655	CB	ALA	225	44.391	20.426	63.346	1.00 14.25	В.
C O	ATOM	1656	C	ALA	225	44.376	21.956	65.332	1.00 16.42	В
60	MOTA	1657	0	ALA	· 225	44.983	21.566	66.329	1.00 14.18	В
	ATOM	1658	N	THR	226	44.385	23.231	64.931	1.00 18.14	В
	MOTA	1659	CA	THR	226	45.135	24.261	65.666	1.00 18.36	В
	MOTA	1660	CB	THR	226	45.205	25.606	64.894	1.00 19.59	В
	MOTA	1661	OG1		226	45.994	25.445	63.705	1.00 20.89	В
65	MOTA	1662	CG2		226	45.821	26.696	65.775	1.00 18.63	В
	ATOM	1663	C	THR	226	44.507	24.541	67.024	1.00 19.56	В
	ATOM	1664	ō	THR	226	45.214	24.765	68.000	1.00 22.00	В
	ATOM	1665	N	LEU	227	43.178	24.527	67.074	1.00 19.70	В
	MOTA	1666	CA	LEU	227	42.427	24.798	68.297	1.00 20.19	В
70	ATOM	1667	CB	LEU	227	41.011	25.291	67.943	1.00 22.99	В
. •	ATOM	1668	CG	LEU	227	40.728	26.794	67.875	1.00 28.11	В
	ATOM	1669		LEU	227	41.162	27.422	69.202	1.00 28.40	В
	ATOM	1670		LEU	227	41.162	27.422	66.677	1.00 27.33	В
	211 011	10,0	-02	550	241	31.475	21.447	00.077	2.00 41.33	

	ATOM	1671	С	LEU	227	42.279	23.627	69.269	1.00 19.64	В
	ATOM	1672	0	LEU	227	42.384	23.801	70.480	1.00 17.11	В
	ATOM	1673	N	MET	228	42.021	22.440	68.727	1.00 21.48	В
	MOTA	1674	CA	MET	228	41.807	21.253	69.557	1.00 21.62	В
5	ATOM	1675	CB	MET	228	40.465	20.627	69.174	1.00 21.31	В
-	MOTA	1676	CG	MET	228	39.286	21.542	69.510	1.00 22.62	В
	ATOM	1677	SD	MET	228	37.764	21.286	68.570	1.00 28.36	В
	MOTA	1678	CE	MET	228	37.979	22.463	67.223	1.00 25.23	В
	ATOM	1679	c	MET	228	42.936	20.235	69.472	1.00 19.55	В
10	MOTA	1680	ŏ	MET	228	43.364	19.884	68.392	1.00 19.08	В
•	MOTA	1681	N	ASN	229	43.404	19.764	70.628	1.00 19.30	В
	ATOM	1682	CA	ASN	229	44.496	1B.790	70.683	1.00 21.72	В
	ATOM	1683	CB	ASN	229	44.902	18.512	72.140	1.00 21.27	В
	ATOM	1684	CG	ASN	229	45.124	19.786	72.952	1.00 23.92	В
15		1685	OD1		229	45.493	20.829	72.413	1.00 26.36	В
13	ATOM				229	44.913	19.694	74.262	1.00 18.44	В
	ATOM	1686	ND2		229		17.460	69.993	1.00 21.18	В
	ATOM	1687	C	ASN		44.165	16.927	70.153	1.00 21.11	В
	ATOM	1688	0	ASN	229	43.071		69.231	1.00 20.55	В
20	MOTA	1689	И	ALA	230	45.129	16.945		1.00 20.33	В
20	ATOM	1690	CA	ALA	230	44.975	15.683	68.510		В
	MOTA	1691	CB	ALA	230	45.172	14.502	69.466 67.869	1.00 22.05	В
	MOTA	1692	С	ALA	230	43.599	15.601			В
	ATOM	1693	0	ALA	230	42.925	14.588	67.974	1.00 23.20	
25	MOTA	1694	N	TYR	231	43.197	16.667	67.191	1.00 20.11	В
25	MOTA	1695	CA	TYR	231	41.878	16.708	66.568	1.00 21.54	В
	MOTA	1696	CB	TYR	231	41.637	18.103	65.968	1.00 19.36	В
	MOTA	1697	CG	TYR	231	40.280	18.276	65.322	1.00 14.20	В
	MOTA	1698		TYR	231	40.106	18.061	63.956	1.00 10.71	В
20	MOTA	1699		TYR	231	38.852	18.173	63.369	1.00 9.05	В
30	MOTA	1700		TYR	231	39.159	18.613	66.085	1.00 14.00	В
	ATOM	1701	CE2	TYR	231	37.900	18.725	65.503	1.00 11.47	В
	MOTA	1702	CZ	TYR	231	37.757	18.505	64.152	1.00 9.28	В
	MOTA	1703	ОН	TYR	231.	36.522	18.626	63.583	1.00 11.26	В
25	MOTA	1704	С	TYR	231	41.603	15.614	65.526	1.00 22.31	В
35	MOTA	1705	0	TYR	231	40.611	14.889	65.630	1.00 23.44	В
	MOTA	1706	N	SER	232	42.481	15.482	64.538	1.00 21.31	В
	ATOM	1707	CA	SER	232	42.286	14.487	63.486	1.00 21.21	В
	MOTA	1708	CB	SER	232	43.382	14.614	62.424	1.00 19.70	В
40	MOTA	1709	OG	SER	232	44.658	14.355	62.980	1.00 22.28	В
40	MOTA	1710	С	SER	232	42.245	13.046	63.983	1.00 20.84	В
	MOTA	1711	0	SER	232	41.718	12.165	63.303	1.00 21.67	В
	ATOM	1712	N	SER	233	42.788	12.805	65.166	1.00 18.82	В
	MOTA	1713	CA	SER	233	42.801	11.447	65.670	1.00 16.78	В
. ~	MOTA	1714	CB	SER	233	44.189	11.108	66.222	1.00 14.92	В
45	MOTA	1715	OG	SER	233	44.295	11.465	67.587	1.00 15.42	B
	MOTA	1716	С	SER	233	41.745	11.193	66.741	1.00 17.60	В
	MOTA	1717	0	SER	233	41.365	10.067	66.964	1.00 18.14	В
	MOTA	1718	N	ARG	234	41.267	12.253	67.392	1.00 18.41	В
	MOTA	1719	CA	ARG	234	40.266	12.113	68.450	1.00 18.22	В
50	MOTA	1720	CB	ARG	234	40.716	12.874	69.703	1.00 20.85	В
	MOTA	1721	CG	ARG	234	41.207	11.975	70.809	1.00 26.63	В
	ATOM	1722	CD	ARG	234	42.603	12.340	71.282	1.00 28.B6	В
	MOTA	·1723	NE	ARG	234	42.624	13.522	72.138	1.00 28.89	В
	MOTA	1724	CZ	ARG	234	43.641	13.853	72.927	1.00 30.32	В
55	MOTA	1725	NH1	ARG	234	44.724	13.089	72.969	1.00 29.87	В
	MOTA	1726	NH2	ARG	234	43.571	14.941	73.683	1.00 29.28	В
	MOTA	1727	С	ARG	234	38.858	12.559	68.065	1.00 18.79	В
	MOTA	1728	0	ARG	234	37.986	12.639	68.914	1.00 18.55	В
	MOTA	1729	N	SER	235	38.641	12.826	66.780	1.00 19.09	· в
60	MOTA	1730	CA	SER	235	37.339	13.278	66.307	1.00 18.40	В
	ATOM	1731	СВ	SER	235	37.477	14.654	65.655	1.00 16.08	В
	ATOM	1732	OG	SER	235	38.275	14.584	64.481	1.00 13.92	В
	MOTA	1733	c	SER	235	36.694	12.314	65.312	1.00 18.89	В
	MOTA	1734	ō	SER	235	37.379	11.637	64.558	1.00 18.57	В
65	ATOM	1735	N	HIS	236	35.363	12.284	65.323	1.00 20.05	В
	MOTA	1736	CA	HIS	236	34.571	11.445	64.427	1.00 20.67	В
	ATOM	1737	CB	HIS	236	33.409	10.800	65.186	1.00 21.89	B
	MOTA .	1738	CG	HIS	236	33.819	10.092	66.439	1.00 22.09	В
	ATOM .	1739		HIS	236	33.733	10.462	67.740	1.00 22.95	В
70	MOTA	1740		HIS	236	34.406	8.847	66.433	1.00 22.44	В
, ,	ATOM	1741		HIS	236	34.663	8.480	67.677	1.00 24.61	В
	MOTA	1742		HIS	236	34.265	9.441	68.489	1.00 23.56	В
	ATOM	1742	C	HIS	236	33.994	12.353	63.345	1.00 21.61	В
	AIUM	1143	C	217	230	22.334	12.333	05.545	1.00 21.01	

•	MOTA	1744	0	HIS	236	33.373	13.368	63.658	1.00 22.50	В
	MOTA	1745	N	SER	237	34.195	12.000	62.080	1.00 20.87	В
	MOTA	1746	CA	SER	237	33.673	12.813	60.992	1.00 21.41	В
_	MOTA	1747	CB	SER	237	34.811	13.241	60.061	1.00 21.79	В
5	MOTA	1748	OG	SER	237	35.388	12.121	59.411	1.00 21.23	В
	MOTA	1749	С	SER	237	32.618	12.049	60.201	1.00 22.61	В
	ATOM	1750		SER	237			59.749		В
			0			32.863	10.939		1.00 23.35	
	HOTA	1751	N	VAL	238	31.440	12.648	60.053	1.00 21.59	В
	MOTA	1752	CA	VAL	238	30.348	12.022	59.313	1.00 20.89	В
10	MOTA	1753	СВ	VAL	238	29.106	11.821	60.234	1.00 22.16	В
	MOTA	1754		VAL	238	28.807	13.104	60.977	1.00 24.21	В
	MOTA	1755	CG2	VAL	238	27.886	11.395	59.419	1.00 18.41	В
	MOTA	1756	С	VAL	238	29.967	12.872	58.103	1.00 18.95	В
	MOTA	1757	0	VAL	238	29.157	13.772	58.205	1.00 18.39	В
15										
13	ATOM	1758	N	PHE	239	30.586	12.577	56.962	1.00 19.38	В
	MOTA	1759	CA	PHE	239	30.329	13.295	55.712	1.00 19.10	В
	MOTA	1760	CB	PHE	239	31.501	13.115	54.735	1.00 16.63	В
	MOTA	1761	CG	PHE	. 239	31.413	13.986	53.501	1.00 13.65	В
	ATOM	1762		PHE	239		13.752			
20						30.443		52.521	1.00 13.62	В
20	ATOM	1763	CD2	PHE	239	32.307	15.029	53.316	1.00 11.10	В
	MOTA	1764	CE1	PHE	239	30.375	14.557	51.367	1.00 11.04	В
	MOTA	1765	CE2	PHE	239	32.248	15.836	52.174	1.00 11.49	В.
	MOTA	1766	cz	PHE	239	31.281	15.598	51.196	1.00 10.13	В
25	MOTA	1767	C	PHE	239	29.072	12.709	55.089	1.00 20.70	· B
23	MOTA	1768	0	PHE	239	29.088	11.581	54.635	1.00 21.65	В
	MOTA	1769	N	SER	240	27.992	13.487	55.056	1.00 19.79	В
	MOTA	1770	CA	SER	240	26.737	12.999	54.489	1.00 20.02	В
	MOTA	1771	CB	SER	240	25.568	13.303	55.430	1.00 17.99	В
	MOTA	1772								
30			OG	SER	240	25.714	12.651	56.682	1.00 13.88	В
30	MOTA	1773	С	SER	240	26.424	13.552	53.104	1.00 21.86	В
	MOTA	1774	0	SER	240	26.721	14.684	52.796	1.00 22.91	В
	ATOM	1775	N	VAL	241	25.818	12.720	52.271	1.00 23.30	В
	ATOM	1776	CA	VAL	241	25.448	13.130	50.932	1.00 24.80	В
35	MOTA	1777	CB	VAL	241	26.432	12.581	49.884	1.00 24.40	В
33	MOTA	1778		VAL	241	26.805	11.139	50.226	1.00 26.22	В
	MOTA	1779	CG2	VAL	241	25.807	12.668	48.494	1.00 19.02	В
	MOTA	1780	C	VAL	241	24.035	12.646	50.619	1.00 26.53	В
	ATOM	1781	0	VAL	241	23.806	11.465	50.433	1.00 27.95	В
	MOTA	1782	N	THR	242	23.093			1.00 28.63	
40							13.582	50.586		В
40	ATOM	1783	CA	THR	242	21.698	13.287	50.311	1.00 30.95	В
	MOTA	1784	CB	THR	242	20.779	14.186	51.164	1.00 32.05	В
	ATOM	1785	0G1	THR	242	20.997	13.901	52.555	1.00 33.54	В
	ATOM	1786	CG2	THR	242	19.319	13.939	50.825	1.00 34.70	В
	ATOM	1787	c	THR	242	21.393	13.490	48.828	1.00 32.32	В
45										
TJ	ATOM	1788	0	THR	242	21.845	14.451	48.213	1.00 33.97	В
	MOTA	1789	N	ILE	243	20.628	12.573	48.250	1.00 33.03	В
	ATOM	1790	CA	ILE	243	20.293	12.660	46.837	1.00 33.83	В
	MOTA	1791	CB	ILE	243	20.912	11.493	46.052	1.00 33.37	В
	MOTA	1792		ILE	243	20.732	11.719	44.561	1.00 32.82	В
50										
50	MOTA	1793		ILE	243	22.395	11.361	46.400	1.00 34.30	В
	MOTA	1794	CDI	ILE	243	23.071	10.176	45.750	1.00 35.23	В
	ATOM	1795	С	ILE	243	18.789	12.635	46.604	1.00 35.12	В
	MOTA	1796	0	ILE	243	18.175	11.581	46.655	1.00 34.29	B
	MOTA	1797	N	HIS	244	18.197	13.803	46.364	1.00 37.02	В
55										
"	MOTA	1798	CA	HIS	244	16.766	13.878	46.097	1.00 38.10	В
	MOTA	1799	CB	HIS	244	16.214	15.280	46.390	1.00 40.10	В
	ATOM	1800	CG	HIS	244	16.190	15.635	47.845	1.00 42.80	В
	MOTA	1801	CD2	HIS	244	15.219	15.493	48.781	1.00 43.38	В
	MOTA	1802	ND1		244	17.271	16.192	48.496	1.00 44.55	В
60										
UU	MOTA	1803		HIS	244	16.968	16.376	49.770	1.00 44.18	В
	MOTA	1804	NE2	HIS	244	15.729	15.960	49.968		В
	MOTA	1805	С	HIS	244	16.569	13.545	44.624	1.00 38.58	В
	ATOM	1806	0	HIS	244	17.113	14.216	43.754	1.00 38.74	В
	ATOM	1807	N	MET	245	15.790	12.500	44.357	1.00 38.78	В
65										
J J	MOTA	1808	CA	MET	245	15.534	12.056	42.991	1.00 38.49	В
	MOTA	1809	CB	MET	245	16.081	10.646	42.791	1.00 35.74	В
	MOTA	1810	CG	MET	245	17.579	10.552	42.978	1.00 34.03	В
	MOTA	1811	SD	MET	245	18.110	8.870	43.218	1.00 32.96	В
	ATOM	1812	CE	MET	245	17.855	8.694	44.996	1.00 26.04	В
70										
, 0	MOTA	1813	C	MET	245	14.058	12.083	42.618	1.00 39.24	B
	MOTA	1814	0	MET	245	13.193	11.814	43.439	1.00 39.24	В
	MOTA	1815	N.	LYS	246	13.791	12.409	41.358	1.00 39.88	В
	MOTA	1816	CA	LYS	246	12.430	12.477	40.855	1.00 40.90	В
				_						_

	MOTA	1817	CB	LYS	246	11.910	13.916	40.915	1.00 42.86	В
	MOTA	1818	CG	LYS	246	10.453	14.080	40.467	1.00 45.41	В
	ATOM	1819	CD	LYS	246	10.140		40.018	1.00 47.23	В
							15.516			
_	NOTA	1820	CE	LYS	246	10.383	16.538	41.134	1.00 49.08	В
5	MOTA	1821	NZ	LYS	246	10.267	17.954	40.659	1.00 47.64	В
	MOTA	1822	C	LYS	246	12.406	11.994	39.414	1.00 41.15	В
										В
	MOTA	1823	0	LYS	246	13.084	12.547	38.552	1.00 40.37	
	MOTA	1824	N	GLU	247	11.622	10.954	39.163	1.00 40.39	В
	MOTA	1825	CA	GLU	247	11.496	10.414	37.821	1.00 40.56	В
10	MOTA	1826	СВ	GLU	247	12.010	8.977	37.769	1.00 39.14	В
10										
	MOTA	1827	CG	GLU	247	11.479	8.090	38.866	1.00 37.23	В
	MOTA	1828	CD	GLU	247	12.390	6.916	39.118	1.00 36.86	В
	HOTA	1829	OE1	GLU	247	12.094	6.104	40.021	1.00 36.22	В
	NOTA	1830		GLU	247	13.410	6.813	38.406	1.00 36.77	В
15										
13	MOTA	1831	С	GŁU	247	10.039	10.469	37.402	1.00 40.31	В
	MOTA	1832	0	GLU	247	9.142	10.304	38.220	1.00 39.86	В
	MOTA	1833	N	THR	248	9.820	10.720	36.117	1.00 40.83	В
	MOTA	1834	CA	THR	248	8.480	10.826	35.569	1.00 40.95	В
	MOTA	1835	CB	THR	248	8.339	12.123	34.736	1.00 40.97	В
20										
20	MOTA	1836		THR	248	8.804	13.238	35.507	1.00 41.15	В
	MOTA	1837	CG2	THR	248	6.886	12.363	34.358	1.00 40.88	В
	ATOM	1838	С	THR	248	8.143	9.625	34.690	1.00 40.36	В
	MOTA	1839	0	THR	248	8.799	9.380	33.684	1.00 40.50	В
	MOTA	1840	N	THR	249	7.111	8.885	35.086	1.00 39.94	В
25										
23	MOTA	1841	CA	THR	249	6.661	7.712	34.341	1.00 39.13	В
	MOTA	1842	CB	THR	249	5.537	6.976	35.086	1.00 39.64	В
	ATOM	1843	OG1	THR	249	4.307	7.686	34.897	1.00 37.39	В
	ATOM	1844	CG2	THR	249	5.846	6.894	36.575	1.00 38.52	В
	MOTA	1845	c	THR	249	6.115	8.132	32.980	1.00 39.50	В
30										
30	MOTA	1846	0	THR	249	5.943	9.311	32.713	1.00 39.71	B
	MOTA	1847	N	ILE	250	5.841	7.148	32.129	1.00 40.73	В
	MOTA	1848	CA	ILE	250	5.307	7.398	30.794	1.00 40.49	В
	MOTA	1849	CB	ILE	250	5.292	6.095	29.944	1.00 37.78	. В
	ATOM	1850		ILE	250	4.244	5.135	30.472	1.00 37.42	В
35										
23	MOTA	1851		ILE	250	4.999	6.421	28.479	1.00 35.79	В
	MOTA	1852	CD1	ILE	250	5.125	5.238	27.552	1.00 33.62	В
	MOTA	1853	С	ILE	250	3.892	7.963	30.905	1.00 42.55	В
	MOTA	1854	0	ILE	250	3.361	8.534	29.953	1.00 43.05	В
	ATOM	1855	N	ASP	251	3.296	7.800	32.084	1.00 44.44	В
40										
40	MOTA	1856	CA	ASP	251	1.947	8.286	32.357	1.00 46.93	В
	MOTA	1857	CB	ASP	251	1.215	7.318	33.290	1.00 47.07	В
	MOTA	1858	CG	ASP	251	0.494	6.221	32.539	1.00 47.33	В
	MOTA	1859	OD1	ASP	251	0.034	5.257	33.190	1.00 47.89	В
	ATOM	1860			251	0.381	6.325	31.298	1.00 45.62	`B
45										
45	MOTA	1861	С	ASP	251	1.965	9.675	32.987	1.00 48.37	В
	ATOM	1862	0	ASP	251	0.933	10.175	33.424	1.00 49.52	В
	MOTA	1863	N	GLY	252	3.145	10.286	33.038	1.00 49.00	В
	MOTA	1864	CA	GLY	252	3.275	11.612	33.609	1.00 48.84	В
	MOTA	1865	c	GLY	252	3.432	11.634	35.117	1.00 49.43	В
50										
20	MOTA	1866	0	GLY	252	3.856	12.638	35.675	1.00 49.95	В
	MOTA	1867	N	GLU	253	3.093	10.538	35.787	1.00 49.54	В
	MOTA	1868	CA	GLU	253	3.219	10.499	37.237	1.00 50.34	В
	ATOM	1869	CB	GLU	253	2.693	9.183	37.797	1.00 51.72	В
	ATOM	1870	CG	GLU	253	2.753	9.136	39.309	1.00 55.44	В
55							7.734	39.856	1.00 57.73	В
55	MOTA	1871	CD	GLU	253	2.605				
	MOTA	1872		GLU		2.703	7.561	41.091	1.00 59.23	В
	MOTA	1873	OE2	GLU	253	2.400	6.805	39.048	1.00 59.21	В
	MOTA	1874	С	GLU	253	4.671	10.678	37.661	1.00 49.73	В
	ATOM	1875	ō	GLU	253	5.582	10.326	36.930	1.00 49.04	В
60										
50	MOTA	1876	N	GLU	254	4.878	11.229	38.851	1.00 49.71	В
	MOTA	1877	CA	GLU	254				1.00 50.40	В
	MOTA	1878	CB	GLU	254	6.452	12.927	39.629	1.00 51.91	В
	ATOM	1879	CG	GLU	254	7.036	13.680	38.448	1.00 56.74	В
	ATOM	1880	CD	GLU	254	6.579	15.124	38.397	1.00 59.63	В
65										
95	ATOM	1881		GLU	254	6.444	15.739	39.479	1.00 61.46	В
	ATOM	1882	OE2	GLU	254	6.363	15.642	37.276	1.00 60.48	В
	MOTA	1883	C	GLU	254	6.562	10.614	40.578	1.00 48.68	В
	ATOM	1884	0	GLU	254	5.812	10.579	41.546	1.00 47.25	В
	MOTA	1885	N	LEU	255	7.703	9.938	40.517	1.00 47.02	В
70									1.00 45.92	
, 0	MOTA	1886	CA	LEU	255	8.157	9.094	41.609		В
	MOTA	1887	CB	LEU	255	8.566	7.722	41.067	1.00 45.31	В
	MOTA	1888	CG	LEU	255	7.647	7.080	40.016	1.00 44.40	В
	MOTA	1889		LEU	255	8.308	5.837	39.454	1.00 43.92	В
		/								_

	ATOM	1890	CD2	LEU	255	6.294	6.747	40.621	1.00 43.09	В
	MOTA	1891	С	LEU	255	9.353	9.780	42.250	1.00 46.31	В
	MOTA	1892	0	LEU	255	10.346	10.044	41.580	1.00 46.88	В
_	MOTA	1893	N	VAL	.256	9.255	10.069	43.545	1.00 46.34	В
5	ATON	1894	CA	VAL	256	10.343	10.739	44.254	1.00 46.32	В
	ATOM	1895	CB	VAL	256	9.837	12.012	44.988	1.00 46.60	В
	ATON .	1896	CG1	VAL	256	9.447	13.075	43.971	1.00 46.43	В
	ATOM	1897	CG2	VAL	256	8.642	11.679	45.870	1.00 46.46	В
	MOTA	1898	С	VAL	256	11.049	9.835	45.258	1.00 45.32	В
10	MOTA	1899	0	VAL	256	10.428	9.287	46.158	1.00 45.96	В
	ATOM	1900	N	LYS	257	12:359	9.687	45.077	1.00 44.55	В
	ATOM	1901	CA	LYS	257	13.190	8.865	45.951	1.00 42.39	В
	MOTA	1902	CB	LYS	257	13.997	7.852	45.133	1.00 43.00	В
	ATOM	1903	CG	LYS	257	13.170	6.932	44.261	1.00 41.72	В
15	ATOM	1904	CD	LYS	257	14.058	6.001	43.457	1.00 38.34	В
	ATOM	1905	CE	LYS	257	14.956	6.771	42.514	1.00 37.62	В
	MOTA	1906	NZ	LYS	257	15.665	5.873	41.563	1.00 37.38	В
	ATOM	1907	С	LYS	257	14.161	9.755	46.705	1.00 40.94	В
	ATOM	1908	0	LYS	257	14.545	10.802	46.220	1.00 42.05	В
20	MOTA	1909	N	ILE	258	14.557	9.322	47.893	1.00 38.70	В
	MOTA	1910	CA	ILE	258	15.498	10.082	48.699	1.00 35.70	В
•	MOTA	1911	CB	ILE	258	14.790	10.816	49.850	1.00 36.93	В.
	MOTA	1912	CG2	ILE	258	15.811	11.596	50.667	1.00 37.53	В
	MOTA	1913	CG1	ILE	258	13.729	11.767	49.291	1.00 38.43	∙B
25	MOTA	1914	CD1	ILE	258	12.932	12.500	50.363	1.00 38.30	В
	MOTA	1915	¢	ILE	25B	16.541	9.142	49.285	1.00 33.73	В
	MOTA	1916	0	ILE	258	16.257	8.388	50.209	1.00 32.97	В
	MOTA	1917	N	GLY	259	17:746	9.186	48.731	1.00 31.67	В
20	MOTA	1918	CA	GLY	259	18.815	8.338	49.219	1.00 30.51	В
30	MOTA	1919	С	GLY	259	19.874	9.136	49.956	1.00 29.55	В
	MOTA	1920	0	GLY	259	20.363	10.138	49.442	1.00 30.38	В
	ATOM	1921	N	LYS	260	20.230	8.692	51.159	1.00 27.15	В
•	MOTA	1922	CA	LYS	260	21.239	9.377	51.958	1.00 26.83	В
25	MOTA	1923	CB	LYS	260	20.603	9.940	53.240	1.00 24.21	В
35	MOTA	.1924	CG	LYS	260	21.518	10.858	54.037	1.00 19.17	В
	ATOM	1925	CD	LYS	260	20.833	11.362	55.289	1.00 17.68	В
	ATOM	1926	CE	LYS	260	21.768	12.219	56.124	1.00 16.42 1.00 16.56	B B
	MOTA	1927	NZ	LYS	260	21.115	12.662	57.378 52.318	1.00 27.97	В
40	ATOM	1928	C	LYS	260	22.394 22.184	8.437 7.357	52.864	1.00 30.85	В
40	MOTA MOTA	1929 1930	N	LYS	260 261	23.616	8.859	52.011	1.00 26.40	В
	ATOM	1931	CA	LEU	261	24.792	8.056	52.306	1.00 24.54	В
	ATOM	1932	CB	LEU	261	25.587	7.830	51.019	1.00 23.41	В
	ATOM	1933	CG	LEU	261	26.989	7.243	51.175	1.00 23.40	В
45	ATOM	1934		LEU	261	26.922	5.920	51.941	1.00 20.72	В
	MOTA	1935		LEU	261	27.599	7.045	49.798	1.00 20.51	В
	ATOM	1936	c	LEU	261	25.685	8.715	53.362	1.00 23.98	В
	ATOM	1937	ŏ	LEU	261	26.117	9.836	53.198	1.00 22.95	В
	ATOM	1938	N	ASN	262	25.953	8.000	54.448	1.00 22.99	В
50	ATOM	1939	CA	ASN	262	26.799	8.529	55.511	1.00 21.81	В
	ATOM	1940	CB	ASN	262	26.138	8.303	56.874	1.00 19.98	В
	MOTA	1941	CC	ASN	262	24.730	8.872	56.945	1.00 24.40	В
	MOTA	1942	OD1	ASN	262	23.770	8.135	57.124	1.00 24.74	В
	MOTA	1943	ND2	ASN	262	24.606	10.189	56.807	1.00 20.69	В
55	MOTA	1944	C	ASN	262	28.192	7.879	55.494	1.00 21.73	В
	MOTA	1945	0	ASN	262	28.314	6.680	55.589	1.00 20.91	В
	ATOM	1946	N	LEU	263	29.238	8.691	55.348	1.00 21.87	В
	ATOM	1947	CA	LEU	263	30.611	8.191	55.338	1.00 20.99	В
	MOTA	1948	CB	LEU	263	31.360	8.750	54.136	1.00 19.60	В
60	MOTA	1949	CG	LEU	263	30.578	8.470	52.856	1.00 20.68	В
	MOTA	1950	CD1	LEU	263	31.187	9.220	51.710	1.00 22.18	В
	MOTA	1951	CD2	LEU	263	30.557	6.972	52.584	1.00 20.91	В
	ATOM	1952	С	LEU	263	31.262	8.650	56.630	1.00 21.08	В
~~	MOTA	1953	0	LEU	263	31.631	9.793	56.753	1.00 20.87	В
65	ATOM	1954	N	VAL	264	31.397	7.734	57.586	1.00 22.31	В
	MOTA	1955	CA	VAL	264	31.964	8.048	58.901	1.00 22.41	В
	MOTA	1956	CB	VAL	264	31.119	7.378	60.042	1.00 22.70	В
	MOTA	1957		VAL	264	31.373	8.082	61.372	1.00 22.08	В
70	MOTA	1958		VAL	264	29.627	7.398	59.691	1.00 23.20	В
70	MOTA	1959	С	VAL	264	33.425	7.645	59.112	1.00 23.23	В
	MOTA	1960	0	VAL	264	33.776	6.482	58.994	1.00 25.35	В
	MOTA	1961	N	ASP	265	34.262	8.625	59.443	1.00 23.36	В
	ATOM	1962	CA	ASP	265	35.683	8.397	59.709	1.00 21.00	В

	MOTA	1963	CB	ASP	265	36.528	9.471	59.011	1.00 17.94	В
	ATOM	1964	CG	ASP	265	38.024	9.311	59.258	1.00 18.29	В
	MOTA	1965		ASP	265	38.429	8.960	60.384	1.00 17.19	В
_	MOTA	1966	OD2	ASP	265	38.806	9.554	58.322	1.00 15.43	В
5	MOTA	1967	С	ASP	265	35.840	8.501	61.230	1.00 21.25	В
	MOTA	1968	0	ASP	265	36.208	9.550	61.758	1.00 22.30	В
					266	35.552	7.406		1.00 19.20	B
	MOTA	1969	N	LEU				61.928		
	MOTA	1970	CA	LEU	266	35.636	7.387	63.387	1.00 19.48	В
	MOTA	1971	CB	LEU	266	35.269	5.991	63.913	1.00 17.26	В
10	ATOM	1972	CG	LEU	266	33.871	5.454	63.567	1.00 18.72	В
				LEU	266		4.005	64.042		В
	MOTA	1973				33.752			1.00 15.87	
	MOTA	1974		LEU	266	32.792	6.332	64.207	1.00 17.11	В
	ATOM	1975	С	LEU	266	37.008	7.818	63.936	1.00 17.95	В
	MOTA	1976	0	LEU	266	37.982	7.938	63.198	1.00 16.50	В
15	ATOM	1977	N	ALA	267	37.053	8.062	65.243	1.00 16.22	В
13										
	MOTA	1978	CA	ALA	267	38.284	8.458	65.920	1.00 17.36	В
	MOTA	1979	CB	ALA	267	37.957	9.144	67.244	1.00 13.49	В
	ATOM	1980	С	ALA	267	39.112	7.202	66.183	1.00 18.67	В
	MOTA	1981	0	ALA	267	38.561	6.119	66.320	1.00 18.45	В
20	MOTA	1982	N	GLY	. 268		7.357	66.249	1.00 18.66	В
20						40.430				
	MOTA	1983	CA	GLY	268	41.291	6.226	66.507	1.00 20.51	В
	MOTA	1984	С	GLY	268	40.738	5.336	67.604	1.00 22.52	В
	ATOM .	1985	0	GLY	268	40.123	5.815	68.545	1.00 22.16	В
	ATOM	1986	N	SER	269	40.974	4.033	67.483	1.00 23.43	В
25		1987		SER	269	40.471	3.075	68.461	1.00 25.19	В
23	MOTA		CA							
	MOTA	1988	CB	SER	269	40.083	1.796	67.750	1.00 24.66	B
	MOTA	1989	OG	SER	269	41.131	1.412	66.883	1.00 25.58	В
	MOTA	1990	С	SER	269	41.446	2.739	69.584	1.00 26.21	В
	MOTA	1991	0	SER	269	41.100	1.996	70.493	1.00 24.37	В
30								69.520		
50	MOTA	1992	N	GLU	270	42.657	3.286		1.00 28.26	В
	ATOM	1993	CA	GLU	270	43.664	3.029	70.546	1.00 31.89	В
	MOTA	1994	CB	GLU	270	45.031	3.589	70.118	1.00 31.04	В
	MOTA	1995	CG	GLU	270	45.140	5.113	70.033	1.00 28.41	В
	MOTA	1996	CD	GLU	270	44.679	5.680	68.701	1.00 28.74	В
35					270			68.471		
55	MOTA	1997		GLU		44.875	6.895		1.00 30.30	В
	MOTA	1998	OEZ	GLU	270	44.129	4.921	67.884	1.00 28.84	В
	MOTA	1999	С	GLU	270	43.262	3.618	71.904	1.00 35.40	В
	MOTA	2000	0	GLU	270	42.847	4.770	71.993	1.00 34.74	В
	ATOM	2001	N	ASN	271	43.378	2,798	72.950	1.00 40.25	В
40										
40	MOTA	2002	CA	ASN	271	43.039	3.192	74.324	1.00 44.12	В
	MOTA	2003	CB	asn	271	41.581	3.693	74.419	1.00 45.82	В
	MOTA	2004	CG	ASN	271	40.546	2.600	74.147	1.00 46.03	В
	ATOM	2005	OD3	ASN	271	39.347	2.845	74.224	1.00 45.22	В
	MOTA	2006		ASN	271	41.011	1.395	73.829	1.00 47.11	В
45										
77	MOTA	2007	C	ASN	271	43.246	2.039	75.307	1.00 45.92	В
	MOTA	2008	0	ASN	271	43.668	0.938	74.922	1.00 46.63	В
	ATOM	2009	N	ASN	287	41.544	11.757	79.480	1.00 56.32	В
	MOTA	2010	CA	ASN	287	40.687	12.175	78.374	1.00 56.59	В
	MOTA	2011	CB	ASN	287	41.514	12.914	77.315	1.00 58.79	В
50										
50	MOTA	2012	CG	ASN	287	42.376	14.006	77.912	1.00 60.93	В
	MOTA	2013	ODl	ASN	287	43.344	13.729	78.617	1.00 62.31	В
	ATOM	2014	ND2	ASN	287	42.024	15.259	77.637	1.00 61.77	В
	MOTA	.2015	С	ASN	287	39.995	10.965	77.736	1.00 54.81	В
	ATOM	2016	ŏ	ASN	287	40.651	10.079	77.181	1.00 55.49	В
55										
33	MOTA	2017	N	ILE	288	38.667	10.940	77.811	1.00 50.95	В
	MOTA	2018	CA	ILE	288	37.889	9.838	77.252	1.00 46.25	В
	MOTA	2019	CB	ILE	288	36.925	9.250	78.314	1.00 48.90	В
	MOTA	2020	CG2	ILE	288	37.713	8.784	79.530	1.00 49.46	В
					288	35.903	10.307	78.741	1.00 49.66	В
60	MOTA	2021		ILE						
00	MOTA	2022	CDI	ILE	288	34.687	9.730	79.435	1.00 51.96	В
	MOTA .	2023	С	ILE	288	37.060	10.259	76.039	1.00 40.91	В
	MOTA	2024	0	ILE	288	36.680	11.423	75.904	1.00 41.77	В
	MOTA	2025	N	ASN	289	36.774	9.302	75.163	1.00 32.95	В
							9.582			
65	MOTA	2026	CA	ASN	289	35.979		73.976	1.00 26.09	В
65	MOTA	2027	CB	ASN	289	36.674	9.045	72.728.	1.00 22.00	В
	MOTA	2028	CG	ASN	289	36.093	9.612	71.444	1.00 19.37	В
	MOTA	2029		ASN	289	36.819	9.927	70.521	1.00 19.84	В
				ASN	289					В
	ATOM	2030				34.774	9.725	71.382	1.00 17.42	
70	MOTA	2031	c	ASN	289	34.624	8.927	74.154	1.00 22.64	В
70	MOTA	2032	Ο.	ASN	289	34.394	7.805	73.718	1.00 22.38	В
	MOTA	2033	N	GLN	290	33.726	9.652	74.806	1.00 20.05	В
	MOTA	2034	CA	GLN	290	32.386	9.166	75.085	1.00 18.94	В
	atom	2035	CB	GLN	290	31.542	10.299	75.659	1.00 20.27	В

	MOTA	2036	CG	GLN	290	30.180	9.847	76.124	1.00 20.13	В
	MOTA	2037	CD	GLN	290	30.273	8.777	77.182	1.00 20.41	В
	ATOM	2038	OEl		290	29.311	8.067	77.441	1.00 22.39	В
	MOTA	2039	NE2		290	31.435	8.662	77.806	1.00 20.99	В
5	MOTA	2040	С	GLN	290	31.652	8.526	73.899	1.00 18.42	В
	ATOM	2041	0	GLN	290	30.945	7.543	74.068	1.00 15.37	В
	ATOM -	2042	N	SER	291	31.808		. 72 . 704	1.00 19.89	В
	MOTA	2043	CA	SER	291	31.139	8.540	71.526	1.00 21.11	В
10	ATOM	2044	CB	SER	291	31.161	9.541	70.366	1.00 22.02	B B
10	ATOM	2045	OG	SER	291	30.121 31.757	10.496 7.212	70.491 71.090	1.00 23.09 1.00 22.87	В
	MOTA MOTA	2046 2047	C O	SER	291 291	31.051	6.294	70.681	1.00 24.87	В
	ATOM	2048	N	LEU	292	33.074	7.107	71.187	1.00 21.56	В
	ATOM	2049	CA	LEU	292	33.741	5.878	70.812	1.00 21.17	В
15	ATOM	2050	CB	LEU	292	35.247	6.097	70.826	1.00 18.31	В
	MOTA	2051	CG	LEU	292	36.074	5.053	.70.089	1.00 18.27	В
	MOTA	2052		LEU	292	35.653	4.994	68.625	1.00 13.66	В
	ATOM	2053		LEU	292	37.548	5.418	70.218	1.00 17.97	B B
20	MOTA	2054	c	LEU	292	33.345 32.914	4.785 3.703	71.818 71.454	1.00 21.64	В
20	MOTA MOTA	2055 2056	0 N	LEU	292 · 293	33.481	5.100	73.098	1.00 22.14	В
	MOTA	2057	CA	LEU	293	33.141	4.172	74.158	1.00 22.23	В
	ATOM	2058	СВ	LEU	293	33.374	4.841	75.513	1.00 22.95	В.
	ATOM	2059	CG	LEU	293	34.479	4.277	76.408	1.00 25.37	В
25	MOTA	2060		LEU	293	35.684	3.860	75.597	1.00 25.32	В
	MOTA	2061		LEU	293	34.851	5.345	77.431	1.00 26.42	В
	MOTA	2062	C	LEU	293	31.689	3.713	74.046	1.00 24.05 1.00 27.12	B B
	MOTA	2063	0	LEU THR	293 294	31:373 30.807	2.552 4.622	74.304	1.00 27.12	В
30	MOTA MOTA	2064 2065	N CA	THR	294	29.396	4.293	73.534	1.00 22.37	В
50	ATOM	2066	СВ	THR	294	28.554	5.580	73.487	1.00 22.35	В
	ATOM	2067		THR	294	28.706	6.277	74.734	1.00 19.68	В
	ATOM	2068	CG2	THR	294	27.090	5.275	73.270	1.00 19.85	В
25	ATOM	2069	C	THR	294	29.148	3.419	72.313	1.00 23.90	В
35	MOTA	.2070	0	THR	294	28.276	2.561	72.325	1.00 26.74	В
	ATOM	2071	N	LEU	295	29.938	3.628	71.268 70.048	1.00 24.08	B B
	MOTA	2072 2073	CA:	LEU	295 295	29.817 30.822	2.846 3.332	69.004	1.00 22.92	В
	ATOM	2074	CG	LEU	295	30.940	2.449	67.760	1.00 22.72	В
40	MOTA	2075		LEU	295	29.647	2.481	66.975	1.00 20.45	В
	ATOM	2076		LEU	295	32.096	2.925	66.907	1.00 22.47	В
	MOTA	2077	С	LEU	295	30.064	1.361	70.340	1.00 26.15	В
	ATOM	2078	0	LEU	295	29.363	0.503	69.836	1.00 28.14	В
45	ATOM	2079	N	GLY	296	31.079	1.076	71.149 71.503	1.00 26.16 1.00 25.55	B B
43	ATOM ATOM	2080 2081	CA	GLY GLY	296 296	31.391 30.300	-0.295 -0.915	72.361	1.00 25.59	В
	ATOM	2082	С О,	GLY	296	29.898	-2.059	72.134	1.00 26.11	В
	ATOM	2083	N	ARG	297	29.817	-0.162	73.346	1.00 22.71	В
	ATOM	2084	CA	ARG	297	28.760	-0.660	74.217	1.00 22.15	В
50	MOTA	2085	CB	ARG	297	28.528	0.306	75.372	1.00 19.27	В
	ATOM	2086	CG	ARG	297	29.719	0.450	76.284	1.00 20.29	В
	ATOM	2087	CD	ARG	297	29.456 30.639	1.467 1.658	77.372 78.201	1.00 22.43	В В
	ATOM ATOM	2088 ⁻ 2089	NE CZ	ARG	297 297	31.226	2.833	78.407	1.00 24.22	В
55	ATOM	2090		ARG	297	30.729	3.921	77.838	1.00 23.11	В
	MOTA	2091		ARG	297	32.306	2.918	79.178	1.00 18.73	В
	ATOM	2092	C	ARG	297	27.449	-0.876	73.452	1.00 21.70	В
	MOTA	2093	0	ARG	297	26.634	-1.674	73.844	1.00 20.12	В
CO	ATOM	2094	N	VAL	298	27.255	-0.138	72.362	1.00 23.14	В
60	MOTA	2095	CA	VAL	298	26.046	-0.284	71.558	1.00 23.54	В
	ATOM	2096	CB	VAL	298	25.845	0.924	70.613	1.00 22.84 1.00 18.86	B B
	MOTA	2097 2098		VAL VAL	298 298	24.742 25.477	0.634 2.146	69.582 71.432	1.00 19.90	В
	ATOM ATOM	2099	C	VAL	298	26.150	-1.563	70.739	1.00 25.65	В
65	MOTA	2100	ō	VAL	298	25.192	-2.325	70.643	1.00 27.92	В
	MOTA	2101	N	ILE	299	27.317	-1.793	70.147	1.00 25.96	В
	ATOM	2102	CA	ILE	299	27.516	-2.992	69.354	1.00 27.94	В
	MOTA	2103	CB	ILE	299	28.880	-2.971	68.649	1.00 26.11	В
70	MOTA	2104		ILE	299	29.187	-4.330	68.053	1.00 24.74	В
70	ATOM	2105		ILE	299	28.862	-1.910	67.550	1.00 26.37	В
	MOTA	2106		ILE	299	30.192	-1.704	66.889	1.00 28.12 1.00 29.09	B
	MOTA	2107	0	ILE	299 299	27.413 26.95B	-4.240 -5.284	70.235 69.791	1.00 28.96	В
	MOTA	2108	J	IUE	233	20.330	-3.204	05.151	1.00 20.70	-

		21.00			200	22 020	4 110	71 400	1 00 20 02	ъ
	MOTA	2109	N	THR	300	27.829	-4.112	71.490	1.00 29.82	В
	MOTA	2110	CA	THR	300	27.771	-5.213	72.440	1.00 30.01	В
	MOTA	2111	CB	THR	300	28.561	-4.877	73.706	1.00 29.27	В
_	MOTA	2112	OG1	THR	300	29.960	-4.842	73.392	1.00 30.68	В
5	MOTA	2113	CG2	THR	300	28.299	-5.900	74.796	1.00 28.12	В
	MOTA	2114	С	THR	300	26.330	-5.517	72.821	1.00 32.39	В
	MOTA	2115	0	THR	300	25.927	-6.675	72.902	1.00 33.67	В
	MOTA	2116	N	ALA	301	25.552	-4.467	73.044	1.00 32.46	В
	ATOH	2117	CA	ALA	301	24.157	-4.631	73.414	1.00 34.19	В
10						23.584	-3.305	73.863	1.00 32.83	В
10	MOTA	2118	СВ	ALA	301					В
	ATOM	2119	С	ALA	301	23.353	-5.182	72.238	1.00 35.75	
	MOTA	2120	0	ALA	301	22.348	-5.842	72.425	1.00 37.02	В
	MOTA	2121	N	LEU	302	23.812	-4.899	71.024	1.00 36.43	В
	ATOM	2122	CA	LEU	302	23.132	-5.352	69.817	1.00 38.14	В
15	ATOM	2123	CB	LEU	302	23.549	-4.488	68.622	1.00 38.00	В
	ATOM	2124	CG	LEU	302	22.492	-3.555	68.031	1.00 39.25	В
	MOTA	2125	CD1	LEU	302	21.823	-2.753	69.128	1.00 39.09	В
	MOTA	2126	CD2	LEU	302	23.149	-2.630	67.016	1.00 38.56	В
	MOTA	2127	С	LEU	302	23.428	-6.812	69.514	1.00 39.23	В
20	ATOM	2128	0	LEU	302	22.520	-7.594	69.249	1.00 39.50	В
	ATOM	2129	N	VAL	303	24.709	-7.163	69.552	1.00 40.87	В
	ATOM.	2130	CA	VAL	303	25.161	-8.521	69.287	1.00 42.58	В
	MOTA	2131	CB	VAL	303	26.706	-8.605	69.331	1.00 42.52	В
							-10.051	69.270	1.00 43.58	В
25	ATOM	2132		VAL	303					8
23	MOTA	2133		VAL	303	27.301	-7.824	68.167	1.00 42.05	
	MOTA	2134	С	VAL	303	24.579	-9.496	70.306	1.00 44.19	В
	MOTA	2135	0	VAL	303		-10.538	69.941	1.00 45.04	В
	ATOM	2136	N	GLU	304	24.685	-9.145	71.584	1.00 45.93	В
~~	MOTA	2137	CA	GLU	304	24.169	-9.973	72.667	1.00 48.10	В
30	ATOM	2138	CB	GLU	304	24.792	-9.541	73.998	1.00 47.26	B
	ATOM	2139	CG	GLU	304	26.305	-9.707	74.041	1.00 46.33	В
	ATOM	2140	CD	GLU	304	26.901	-9.334	75.382	1.00 46.65	В
	ATOM	2141		GLU	304	28.139	-9.410	75.519	1.00 44.41	В
	ATOM	2142		GLU	304	26.135	-8.968	76.302	1.00 47.42	В
35	MOTA	2143	c	GLU	304	22.649	-9.885	72.753	1:00 49.92	В
	ATOM	2144	ō	GLU	304		-10.492	73.612	1.00 50.02	В
	ATOM	2145	N	ARG	305	22.061	-9.116	71.844	1.00 52.91	В
	ATOM	2146	CA	ARG	305	20.614	-8.941	71.787	1.00 56.32	В
		2147		ARG	305		-10.251	71.357	1.00 58.76	B
40	MOTA		CB						1.00 63.36	В
40	ATOM	2148	CG	ARG	305		-10.652	69.934		В
	MOTA	2149	CD	ARG	305		-11.856	69.475	1.00 68.00	
	MOTA	2150	NE	ARG	305		-12.133	68.057	1.00 71.78	В
	MOTA	2151	CZ	ARG	305		-11.344	67.068	1.00 73.93	В
15	ATOM	2152		ARG	305		-10.222	67.339	1.00 74.69	·B
45	MOTA	2153		ARG	305		-11.675	65.807	1.00 75.22	В
	MOTA	2154	С	ARG	305	19.981	-8.443	73.082	1.00 56.68	В
	ATOM	2155	0	ARG	305	18.809	-8.699	73.340	1.00 56.68	В .
	MOTA	2156	N	THR	306	20.757	-7.728	73.892	1.00 57.02	В
	MOTA	2157	CA	THR	306	20.248	-7.185	75.146	1.00 56.82	В
50	MOTA	2158	CB	THR	306	21.347	-6.426	75.912	1.00 56.33	В
	ATON	2159	OG1	THR	306	22.482	-7.281	76.095	1.00 56.76	В
	MOTA	2160		THR	306	20.836	-5.975	77.272	1.00 56.64	В
	MOTA	2161	C	THR	306	19.122	-6.213	74.812	1.00 57.35	В
	ATOM	2162	ō	THR	306	19.239	-5.421	73.881	1.00 58.12	В
55	ATOM	2163	N	PRO	307	18.011	-6.268	75.564	1.00 57.68	В
-	MOTA	2164	CD		. 307	17.750	-7.184	76.688	1.00 58.36	В
							-5.384	75.336	1.00 57.69	В
	MOTA	2165	CA	PRO	307	16.861			1.00 57.98	В
	MOTA	2166	CB	PRO	307 ·	15.959	-5.682	76.533		
60	MOTA	2167	CG	PRO	307	16.241	-7.125	76.803	1.00 58.68	В
60	ATOM	2168	¢	PRO	307	17.218	-3.898	75.237	1.00 56.99	В
	ATOM	2169	0	PRO	307	16.684		74.386		В
	MOTA	2170	N	HIS	308	18.120	-3.439	76.105	1.00 55.27	В
	MOTA	2171	CA	HIS	308	18.539	-2.034	76.123	1.00 53.51	В
	ATOM	2172	CB	HIS	308	18.749	-1.565	77.567	1.00 55.71	₿.
65	ATOM	2173	CG	HIS	308	19.227	-0.150	77.677	1.00 58.12	В
	ATOM	2174		HIS	308	20.385	0.367	78.155	1.00 59.12	В
	ATOM	2175		HIS	308	18.475	0.925	77.252	1.00 58.97	В
	ATOM	2176		HIS	308	19.148	2.043	77.464	1.00 58.91	В
	ATOM	2177		HIS	308	20.310	1.732	78.012	1.00 59.24	В
70	MOTA	2178		HIS	308	19.813	-1.749	75.329	1.00 50.82	. в
, ,			C						1.00 50.82	В
	ATOM	2179	0	HIS	308	20.793	-2.472	75.433		
	ATOM	2180	N	VAL	309	19.780	-0.671	74.551	1.00 47.79	B
	MOTA	2181	CA	VAL	309	20.921	-0.239	73.743	1.00 44.18	В

	MOTA	2182	CB	VAL	309	20.619	-0.355	72.233	1.00 44.37	В
	MOTA	2183		VAL	309	21.876	-0.067	71.427	1.00 43.69	В
					309	20.076	-1.737	71.912	1.00 43.50	В
	MOTA	2184		VAL						
_	MOTA	2185	С	VAL	309	21.188	1.234	74.075	1.00 41.50	В
5	MOTA	2186	0	VAL	309	20.368	2.091	73.788	1.00 41.50	В
	MOTA	2187	N	PRO	310	22.351	1.535	74.675	1.00 38.54	В
		2188		PRO	310	23.440	0.586	74.968	1.00 37.32	В
	ATOM-		CD							
	MOTA	2189	CA	PRO	310	22.736	2.898	75.058	1.00 37.55	В
	MOTA	2190	CB	PRO	310	23.983	2.669	75.909	1.00 36.77	В
10	MOTA	2191	CG	PRO	310	24.614	1.502	75.238	1.00 36.14	В
	MOTA	2192	c	PRO	310	22.977	3.898	73.917	1.00 36.95	В
									1.00 36.57	В
	MOTA	2193	0	PRO	310	24.042	4.493	73.827		
	MOTA	2194	N	TYR	311	21.972	4.076	73.061	1.00 36.05	В
	MOTA	2195	CA	TYR	311	22.047	5.012	71.940	1.00 34.95	В
15	MOTA	2196	CB	TYR	311	20.778	4.949	71.085	1.00 35.41	В
	MOTA	2197	CG	TYR	311	20.603	3.711	70.245	1.00 36.70	В
									1.00 35.89	В
	MOTA	2198		TYR	311	21.603	3.289	69.374		
	MOTA	2199	CE1	TYR	311	21.433	2.161	68.578	1.00 36.91	В
	MOTA	2200	CD2	TYR	311	19.416	2.973	70.300	1.00 36.75.	В
20	ATOM	2201		TYR	311 ·	19.234	1.844	69.508	1.00 36.61	В
	ATOM	2202	cz	TYR	311	20.247	1.442	68.651	1.00 36.85	В
	ATOM	2203	он	TYR	311	20.086	0.312	67.882	1.00 35.56	В.
	MOTA	2204	С	TYR	311	22.217	6.462	72.402	1.00 35.12	В
	MOTA	2205	0	TYR	311	23.038	7.186	71.868	1.00 34.13	· B
25	ATOM	2206	N	ARG	312	21.422	6.868	73.392	1.00 34.48	В
	MOTA	2207	CA	ARG	312	21.444	8.237	73.906	1.00 34.28	В
	ATOM	2208	CB	ARG	312	20.160	8.523	74.690	1.00 35.83	В
	MOTA	2209	CG	ARG	312	18.882	8.227	73.935	1.00 41.17	В
	ATOM	2210	CD	ARG	312	17.732	8.007	74.897	1.00 44.62	В
30	MOTA	2211	NE	ARG	312	16.596	7.341	74.263	1.00 48.42	В
	ATOM	2212	cz	ARG	312	15.608	6.747	74.926	1.00 51.08	В
								76.254	1.00 50.32	В
	ATOM	2213		ARG	312	15.610	-6.732			
	MOTA	2214	NH2	ARG	312	14.618	6.163	74.259	1.00 51.58	В
	ATOM	2215	С	ARG	312	22.638	8.593	74.787	1.00 33.03	В
35	MOTA	.2216	0	ARG	312	22.701	9.699	75.317	1.00 34.26	В
	MOTA	2217	N	GLU	313	23.581	7.669	74.953	1.00 29.69	В
						24.735	7.947	75.799	1.00 25.30	В
	ATOM	2218	CA	GLU	313					
	MOTA	2219	CB	GLU	313	25.200	6.655	76.481	1.00 24.49	В
	MOTA	2220	CG	GLU	313	24.278	6.242	77.634	1.00 25.08	В
40	ATOM	2221	CD	GLU	313	24.677	4.946	78.327	1.00 23.59	В
	ATOM	2222		GLU	313	25.883	4.722	78.553	1.00 23.79	В
							4.156	78.665	1.00 23.87	В
	MOTA	2223		GLU	313	23.775				
	MOTA	2224	C	GLU	313	25.898	8.646	75.089	1.00 23.89	В
	MOTA	2225	0	GLU	313	26.963	8.806	75.659	1.00 23.12	В
45	ATOM	2226	N	SER	314	25.680	9.068	73.843	1.00 21.70	В
	MOTA	2227	CA	SER	314	26.714	9.766	73.080	1.00 21.61	В
	MOTA	2228	СВ	SER	314	27.800	8.796	72.622	1.00 19.78	В
										B
	MOTA	2229	OG	SER	314	27.401	8.118	71.442	1.00 17.85	
	MOTA	2230	С	SER	314	26.124	10.466	71.861	1.00 23.50	В
50	MOTA	2231	0	SER	314	25.047	10.105	71.388	1.00 23.43	В
	ATOM	2232	N	LYS	315	26.840	11.462	71.348	1.00 23.77	В
	ATOM	2233	CA	LYS	315	26.367	12.204	70.186	1.00 24.56	В
			CB	LYS			13.462	69.963	1.00 24.98	B
	MOTA	2234			315	27.216				
	MOTA	2235	CG	LYS	315	27.295	14.394	71.165	1.00 25.63	В
55	MOTA	2236	CD	LYS	315	.25.926	14.862	71.607	1.00 25.73	В
	ATOM	2237	CE	LYS	315	26.034	15.834	72.774	1.00 26.31	В
	MOTA	2238	NZ	LYS	315	26.660	17.123	72.353	1.00 30.29	В
				LYS		26.416		68.939	1.00 24.22	В
	ATOM	2239	C		315		11.335			
60	MOTA	2240	0	LYS	315	25.498	11.338	68.138	1.00 25.98	В
60	MOTA	2241	N	LEU	316	27: 503	10.591	68.78 7	1.00 23.22	В
	ATOM	2242	CA	LEU	316	27.674	9.719	67.636	1.00 24.18	В
	ATOM	2243	CB	LEU	316	29.039	9.022	67.711	1.00 24.13	В
		2244						66.488	1.00 23.55	В
	ATOM		CG	LEU	316	29.451	8.205			
	MOTA	2245		LEU	316	29.850	9.149	65.370	1.00 25.34	В
65	ATOM	2246	CD2	LEU	316	30.609	7.299	66.840	1.00 22.84	В
	MOTA	2247	С	LEU	316	26.567	8.664	67.506	1.00 23.18	В
	MOTA	2248	ŏ	LEU	316	25.892	8.590	66.480	1.00 22.77	В
	MOTA	2249	N	THR	317	26.369	7.855	68.543	1.00 22.09	В
70	MOTA	2250	CA	THR	317	25.346	6.817	68.470	1.00 22.50	В
70	ATOM	2251	CB	THR	317	25.459	5.809	69.651	1.00 20.87	В
	MOTA	2252		THR	317	25.198	6.472	70.892	1.00 19.26	В
				THR	317	26.848	5.192	69.682	1.00 20.16	В
	ATOM	2253								
	MOTA	2254	С	THR	317	23.923	7.367	68.394	1.00 23.49	В

	MOTA	2255	0	THR	317	23.025	6.684	67.929	1.00 23.95	В
	MOTA	2256	N	ARG	318	23.723	8.606	68.836	1.00 23.82	В
	ATOM	2257	CA	ARG	318	22.402	9.225	68.764	1.00 25.01	В
	ATOM	2258	CB	ARG	318	22.317	10.426	69.705	1.00 28.63	В
5				ARG	318	21.923	10.065	71.120	1.00 34.53	В
,	MOTA	2259	CG				11.179	72.094	1.00 38.92	В
	MOTA	2260	CD	ARG	318	22.260				В
	MOTA	2261	NE	ARG	318	21.606	12.436	71.745	1.00 45.13	
	MOTA	2262	CZ	ARG	318	20.293	12.642	71.792	1.00 47.64	В
10	MOTA	2263	NH1		318	19.479		72.177	1.00 49.68	В
10	MOTA	2264	NH2		318	19.796	13.826	71.456	1.00 45.41	В
	MOTA	2265	С	ARG	318	22.127	9.674	67.335	1.00 24.81	В
	MOTA	2266	0	ARG	318	21.015	9.522	66.828	1.00 24.93	В
	MOTA	2267	N	ILE	319	23.149	10.217	66.684	1.00 22.86	В
	MOTA	2268	CA	ILE	319	23.001	10.688	65.313	1.00 23.60	В
15	MOTA	2269	CB	ILE	319	24.197	11.588	64.893	1.00 22.37	В
	MOTA	2270	CG2	ILE	319	24.089	11.947	63.410	1.00 22.84	В
	ATOM	2271	CG1	ILE	319	24.224	12.861	65.748	1.00 22.76	В
	ATOM	2272		ILE	319	25.457	13.738	65.533	1.00 17.34	В
	MOTA	2273	c	ILE	319	22.903	9.532	64.322	1.00 24.40	В
20	ATOM	2274	ŏ	ILE	319	22.144	9.585	63.381	1.00 23.60	В
-0	MOTA	2275	N	LEU	320	23.688	8.486	64.556	1.00 27.00	В
	ATOM	2276	CA	LEU	320	23.725	7.331	63.664	1.00 28.83	В
		2277		LEU	320	25.180	7.037	63.274	1.00 26.75	В
	ATOM		CB		320	26.035	8.151	62.668	1.00 28.19	В
25	ATOM	2278	CG	LEU			7.720	62.710	1.00 27.81	В
23	MOTA	2279		LEU	320	27.479			1.00 26.81	В
	MOTA	2280		LEU	320	25.601	8.459 6.053	61.237	1.00 30.42	В
	MOTA	2281	C	LEU	320	23.098		64.220 63.841	1.00 30.42	B
	MOTA	2282	0	LEU	320	23.501	4.957			В
20	MOTA	.2283	N	GLN	321	22.097	6.188	65.085	1.00 32.73	В
30	MOTA	2284	CA	GLN	321	21.457	5.012	65.674	1.00 34.42	
	MOTA	2285	CB	GLN	321	20.466	5.419	66.777	1.00 35.23	В
	MOTA	2286	CG	GLN	321	19.195	6.116	66.314	1.00 39.71	В
	MOTA	2287	CD	GLN	321	18.320	6.569		. 1.00 42.32	В
25	MOTA	2288		GL10	321	17.881	5.755	68.298	1.00 42.09	В
35	MOTA	2289		GLN	321	18.069	7.877	67.577	1.00 44.14	В
	MOTA	2290	С	GLN	321	20.758	4.102	64.663	1.00 33.44	B
	MOTA	2291	0	GLN	321	20.677	2.901	64.868	1.00 34.48	В
	MOTA	2292	N	ASP	322	20.261	4.666	63.569	1.00 32.24	В
40	MOTA	2293	CA	ASP	322	19.583	3.839	62.575	1.00 33.02	В
40	MOTA	2294	CB	ASP	322	18.780	4.693	61.595	1.00 32.22	В
	MOTA	2295	CG	ASP	322	17.790	3.871	60.783	1.00 32.38	В
	ATOM	2296	OD1	ASP	322	17.716	4.061	59.548	1.00 32.08	В
	ATOM	2297	OD2	ASP	322	17.074	3.045	61.382	1.00 30.54	В
	MOTA	2298	С	ASP	322	20.598	3.011	61.794	1.00 32.49	В
45	ATOM	2299	ο.	ASP	322	20.228	2.175	60.988	1.00 32.45	В
	MOTA	2300	N	SER	323	21.880	3.274	62.030	1.00 32.77	В
	MOTA	2301	CA	SER	323	22.951	2.547	61.361	1.00 30.97	В
	ATOM	2302	CB	SER	323	24.122	3.480	61.067	1.00 28.95	В
	MOTA	2303	OG	SER	323	23.837	4.320	59.959	1.00 27.41	В
50	MOTA	2304	С	SER	323	23.416	1.374	62.224	1.00 30.75	В
	MOTA	2305	0	SER	323	24.171	0.517	61.783	1.00 29.17	В
	ATOM	2306	N	LEU	324	22.966	1.352	63.470	1.00 30.45	В
	ATOM	-2307	CA	LEU	324	23.326	0.270	64.363	1.00 31.28	В
	ATOM	2308	CB	LEU	324	24.046	0.809	65.606	1.00 31.28	В
55	MOTA	2309	CG	LEU	324	25.476	1.353	65.463	1.00 32.14	В
	ATOM	2310			. 324	26.308	0.424	64.587	1.00 33.04	В
	ATOM	2311		LEU	324	25.436	2.739	64.862	1.00 34.26	B
	ATOM	2312	c	LEU	324	22.081	-0.511	64.771	1.00 31.54	В
	ATOM	2313	ŏ	LEU	324	21.468	-0.235	65.785	1.00 31.30	. в
60		2314	N	GLY	325	21.715	-1.490	63.950	1.00 33.73	8
UU	ATOM				325	20.554	-2.311	64.249	1.00 33.79	В
	ATOM	2315	CA	GLY						В
	MOTA	2316	C	CLY	325	19.244	-1.636	63.901	1.00 33.20	
	MOTA	2317	0	GLY	325	18.218	-1.905	64.517	1.00 33.16	B
65	MOTA	2318	N	GLY	326	19.286	-0.754	62.909	1.00 32.43	B
65	MOTA	2319	CA	GLY	326	18.090	-0.048	62.499	1.00 33.13	9
	MOTA	2320	C	GLY	326	17.704	-0.420	61.088	1.00 34.86	В
	ATOM	2321	0	GLY	326	17.905	-1.541	60.680	1.00 34.93	В
	MOTA	2322	N	ARG	327	17.157	0.535	60.343	1.00 37.13	В
70	MOTA	2323	CA	ARG	327	16.748	0.278	58.974	1.00 38.94	В
70	MOTA	2324	CB	ARG	327	15.327	0.784	58.753	1.00 43.05	. В
	MOTA	2325	CG	ARG	327	14.278	0.034	59.559	1.00 49.59	В
	MOTA	2326	CD	ARG	327	12.872	0.464	59.159	1.00 54.64	В
	MOTA	2327	NE	ARG	327	12.071	-0.657	58.665	1.00 60.40	В

	ATOM	2328	CZ	ARG	327	12.358	-1.380	57.583	1.00 62.77	В
	ATOM	2329	NH1		327	13.441	-1.105	56.861	1.00 63.46	В
	ATOM	2330	NH2		327	11.556	-2.377	57.219	1.00 61.73	В
		2331		ARG	327	17.686	0.887	57.934	1.00 38.03.	В
5	MOTA			ARG	327	17.249	1.289	56.869	1.00 37.61	В
)	MOTA	2332				18.979	0.931	58.252	1.00 36.37	В
	MOTA	2333		THR	328			57.345	1.00 35.54	В
	ATOM	2334		THR	328	19.983	1.481			В
	MOTA	2335	-	THR	328	20.715	2.685	57.989	1.00 34.89	
10	MOTA	2336	OG1		328	19.798	3.762	58.194	1.00 35.66	В
10	ATOM	2337	CG2	THR	328	21.847	3.156	57.096	1.00 33.72	В
	MOTA	2338	С	THR	328	21.040	0.442	56.974	1.00 34.98	В
	MOTA	2339	0	THR	328	21.630	-0.170	57.848	1.00 36.65	В
	MOTA	2340	N	ARG	329	21.274	0.252	55.678	1.00 33.43	В
	MOTA	2341	CA	ARG	329	22.281	-0.704	55.226	1.00 33.67	B
15	ATOM	2342	CB	ARG	329	22.354	-0.752	53.696	1.00 35.61	B
	MOTA	2343	CG	ARG	329	23.146	-1.938	53.156	1.00 40.29	В
	MOTA	2344		ARG	329	23.642	-1.691	51.736	1.00 45.76	В
	ATOM	2345		ARG	329	24.253	-2.877	51.133	1.00 51.83	В
	ATOM	2346	CZ	ARG	329	25.297	-3.540	51.632	1.00 54.83	В
20	ATOM	2347	NH1		329	25.874	-3.148	52.761	1.00 54.64	В
20	MOTA	2348	NH2		329	25.772	-4.601	50.991	1.00 56.00	В
	ATOM	2349	C	ARG	329	23.615	-0.218	55.764	1.00 30.92	В.
		2350		ARG	329	24.034	0.871	55.452	1.00 33.46	В
	MOTA		0			24.277	-1.028	56.573	1.00 28.10	В
25	MOTA	2351		THR	330			57.156	1.00 26.64	В
23	ATOM	2352	CA	THR	330	25.541	-0.622	58.691	1.00 25.12	В
	ATOM	2353	CB	THR	330	25.410	-0.524		1.00 25.09	В
	ATOM	2354	OG1		330	24.526	0.549	59.019		В
	MOTA	2355	CG2		330	26.760	-0.291	59.351	1.00 22.76	В
20	MOTA	2356	С	THR	330	26.723	-1.516	56.820	1.00 27.27	
30	MOTA	2357	0	THR	330	26.602	-2.732	56.748	1.00 27.57	В
	MOTA	2358	N	SER	331	27.868	-0.878	56.618	1.00 26.82	В
	MOTA	2359	CA	SER	331	29.104	-1.567	56.308	1.00 26.67	В
	MOTA	2360	CB	SER	331	29.442	-1.446	54.830	1.00 26.29	В
	MOTA	2361	OG	SER	331	28.444	-2.072	54.052	1.00 31.25	В
35	MOTA	· 2362	С	SER	331	30.191	-0.907	57.125	1.00 26.05	В
	MOTA	2363	0	SER	331	30.210	0.304	57.272	1.00 29.07	В
	ATOM	2364	N	ILE	332	31.086	-1.712	57.677	1.00 24.35	В
	MOTA	2365	CA	ILE	332	32.179	-1.190	58.472	1.00 20.58	B
	ATOM	2366	СВ	ILE	332	32.119	-1.704	59.917	1.00 16.78	В
40	ATOM	2367	CG2		332	33.367	-1.290	60.656	1.00 15.30	В
	ATOM	2368	CG1		332	30.849	-1.195	60.605	1.00 14.73	В
	MOTA	2369	CD1		332	30.641	-1.735	62:018	1.00 11.20	В
	MOTA	2370	c	ILE	332	33.484	-1.646	57.855	1.00 22.60	В
	MOTA	2371	ŏ	ILE	332	33.635	-2.809	57.495	1.00 22.21	В
45	ATOM	2372	N	ILE	333	34.421	-0.718	57.713	1.00 23.08	В
73	ATOM	2373	CA	ILE	333	35.718	-1.046	57.148	1.00 21.26	В
		2374		ILE	333	36.096	-0.086	56.011	1.00 20.77	В
	MOTA		CB	ILE	333	37.401	-0.530	55.375	1.00 20.19	B
	MOTA	2375				34.993	-0.065	54.950	1.00 22.76	В
50	ATOM	2376		ILE	333		0.826	53.738	1.00 19.77	В
20	ATOM	2377		ILE	333	35.297	-0.927	58.267	1.00 22.44	В
	MOTA	2378	C	ILE	333	36.736		58.740	1.00 25.05	В
	MOTA	2379	0	ILE	333	37.015	0.170		1.00 22.25	В
	MOTA	2380	N	ALA	334	37.269	-2.061	58.708		В
~ ~	MOTA	2381	CA	ALA	334	38.252	-2.080	59.783	1.00 21.24	
55	MOTA	2382	CB	ALA	334	38.088	-3.351	60.605	1.00 21.16	В
	MOTA	2383	С	ALA	334	39.667	-1.998	59.212	1.00 20.54	В
	ATOM	2384	0	ALA	334	40.070	-2.850	58.452	1.00 21.75	В
	MOTA	2385	N	THR	335	40.405	-0.952	59.582	1.00 18.02	В
	MOTA	2386	CA	THR	335	41.772	-0.771	59.102	1.00 15.52	₿
60	MOTA	2387	CB	THR	335	42.052	0.701	58.752	1.00 14.93	В
	MOTA	2388	OG1	THR	335	41.551	1.558	59.794	1.00 16.56	B
	MOTA	2389		THR	335	41.394	1.051	57.447	1.00 13.76	В
	MOTA	2390	С	THR	335	42.780	-1.257	60.132	1.00 14.40	В
	ATOM	2391	ō	THR	335	42.586	-1.096	61.340	1.00 13.68	В
65	ATOM	2392	N	ILE	336	43.863	-1.849	59.641	1.00 15.75	В
03		2393	CA	ILE	336	44.893	-2.409	60.506	1.00 16.07	В
	ATOM		CB	ILE	336	44.671	-3.936	60.702	1.00 14.75	В
	MOTA	2394		ILE		43.346	-4.185	61.401	1.00 13.27	В
	MOTA	2395			336				1.00 15.22	В
70	MOTA	2396		ILE	336	44.678	-4.662	59.348	1.00 13.22	B
70	MOTA	2397		ILE	336	44.726	-6.215	59.461		
	MOTA	2398	c	ILE	336	46.317	-2.186	59.999	1.00 17.99	В
	MOTA	2399	0	ILE	336	46.534	-1.816	58.844	1.00 17.06	В
	MOTA	2400	И	SER	337	47.280	-2.407	60.889	1.00 20.83	В

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	MOTA	2401	CA	SER	337 337	48.694	-2.250	60.570 61.685	1.00 23.58 1.00 22.57	B B
	MOTA MOTA	2402 2403	CB OG	SER SER	337	49.399 50.792	-1.491 -1.737	61.645	1.00 21.86	В
	ATOM	2404	c	SER	337	49.395	-3.600	60.389	1.00 27.32	В
5	ATOM	2405	ŏ	SER	337	49.123	-4.548	61.122	1.00 27.36	В
	MOTA	2406	N	PRO	338	50.320	-3.688	59.416	1.00 28.03	В
	MOTA	2407	CD	PRO	338	50.612	-2.678	58.383	1.00 29.38	В
	MOTA	2408	CA	PRO	338	51.063	-4.919	59.147	1.00 30.56	В
10	MOTA	2409	CB	PRO	338	51.485	-4.743	57.698	1.00 29.47	B B
10	MOTA	2410	CG	PRO PRO	338 338	51.804 52.274	-3.283 -5.047	57.657 60.074	1.00 28.23	В
	MOTA MOTA	2411 2412	C 0	PRO	338	52.903	-6.083	60.131	1.00 32.55	В
	MOTA	2413	N	ALA	339	52.586	-3.972	60.790	1.00 33.15	В
	MOTA	2414	CA	ALA	339	53.732	-3.955	61.690	1.00 34.44	В
15	MOTA	2415	CB	ALA	339	54.051	-2.518	62.109	1.00 35.58	В
	MOTA	2416	С	ALA	339	53.505	-4.816	62.918	1.00 35.05	. В
	MOTA	2417	0	ALA	339	52.391	-4.956	63.386	1.00 35.58	B B
	MOTA	2418 2419	N CA	SER SER	340 340	54.585 54.479	-5.380 -6.236	63.447 64.615	1.00 36.42	В
20	MOTA MOTA	2420	CB	SER	340	55.694	-7.162	64.717	1.00 36.55	В
20	MOTA	2421	OG	SER	340	56.891	-6.431	64.909	1.00 37.23	В
	MOTA	2422	C	SER	340	54.324	-5.457	65.914	1.00 36.18	В
	ATOM	2423	0	SER	340	53.769	-5.969	66.B71	1.00 36.17	В
25	ATOM	2424	N	LEU	341	54.803	-4.220	65.957	1.00 36.13	В
25	MOTA	2425	CA	LEU	341	54.664 55.663	-3.453 -2.296	67.190 67.239	1.00 38.21	. B
	ATOM ATOM	2426 2427	CB CG	LEU	341 341	55.293	-1.011	66.500	1.00 44.27	В
	ATOM	2428		LEU	341	56.054	0.160	67.121	1.00 44.94	В
	MOTA	2429		LEU	341	55.597	-1.158	65.011	1.00 45.97	В
30	MOTA	2430	C	LEU	341	53.244	-2.912	67.337	1.00 36.82	В
	MOTA	2431	0	LEU	341	52.944	-2.185	68.259	1.00 37.65	В
	MOTA	2432	N	ASN	342	52.376	-3.288	66.408	1.00 36.59	B B
	MOTA	2433 2434	CA CB	ASN ASN	342 342	50.983 50.636	-2.856 -2.219	66.416 65.071	1.00 34.64	В
35	MOTA MOTA	2435	œ	ASN	342	51.343	-0.903	64.865	1.00 34.11	В
	MOTA	2436		ASN	342	51.904	-0.649	63.808	1'.00 32.85	В
	ATOM	2437		ASN	342	51.315	-0.052	65.888	1.00 32.94	В
	MOTA	2438	С	ASN	342	50.084	-4.048	66.661	1.00 35.91	В
40	MOTA	2439	0	ASN	342	48.860	-3.958	66.561	1.00 37.26	B B
40	MOTA	2440	N	LEU LEU	343 343	50.720 50.033	-5.164 -6.419	66.993 67.244	1.00 34.56	В
	ATOM ATOM	2441 2442	CA CB	LEU	343	51.019	-7.433	67.836	1.00 31.23	В
	MOTA	2443	ÇG	LEU	343	50.546	-8.858	68.135	1.00 31.25	В
	MOTA	2444		LEU	343	50.001	-8.944	69.548	1.00 32.82	В
45	MOTA	2445		LEU	343	49.504	-9.286	67.101	1.00 30.64	В
	MOTA	2446	C	LEU	343	48.817	-6.295	68.140 67.732	1.00 30.37	B B
	MOTA MOTA	2447 2448	О И	LEU GLU	343 344	47.714 49.023	-6.608 -5.831	69.364	1.00 30.64	В
	MOTA	2449	CA	GLU	344	47.922	-5.710	70.307	1.00 32.19	В
50	MOTA	2450	CB	GLU	344	48.442	-5.121	71.619	1.00 34.78	В
	MOTA	2451	CG	GLU	344	47.460	-5.189	72.761	1.00 42.18	В
	MOTA	2452	CD	GLU	344	48.107	-4.861	74.099	1.00 47.80	В
	MOTA	2453		GLU	344	48.743	-3.785	74.209	1.00 48.41	. B
55	MOTA MOTA	2454 2455	C C	GLU	344 344	47.982 46.736	-5.686 -4.899	75.036 69.760		. B
"	MOTA	2456	ò	GLU	344	45.600	-5.355	69.802	1.00 29.53	. B
	ATOM	2457	N	GLU	345	46.991	-3.707	69.234	1.00 29.30	В
	MOTA	2458	CA	GLU	345	45.901	-2.891	68.703	1.00 29.30	В
	MOTA	2459	CB	GLU	345	46.393	-1.477	68.349	1.00 29.27	. В
60	MOTA	2460	CC	GLU	345	46.618	-0.581	69.565	1.00 29.72	В
	MOTA	2461	CD	GLU	345	45.337	-0.285	70.330	1.00 30.47	B
	ATOM	2462		GLU	345 345	45.429 44.241	0.193 -0.521	71.482 69.786	1.00 30.71	В
	MOTA MOTA	2463 2464	C C	GLU	345	45.277	-3.556	67.476	1.00 27.38	B
65	MOTA	2465	ō	CLU	345	44.082	-3.423	67.233	1.00 28.53	В
	ATOM	2466	N	THR	346	46.084	-4.283	66.711	1.00 24.59	В
	MOTA	2467	CA	THR	346	45.576	-4.979	65.530	1.00 23.55	В
	MOTA	2468	CB	THR	346	46.717	-5.588	64.721	1.00 22.82	В
70	MOTA	2469		THR	346	47.503	-4.534	64.147	1.00 24.62	B B
10	MOTA MOTA	2470 2471		THR THR	346 346	46.173 44.597	-6.473 -6.083	63.618 65.937	1.00 23.82	В
	ATOM	2472	C D	THR	346	43.617	-6.343	65.252	1.00 22.38	В
	ATOM	2473	N	LEU	347	44.873	-6.732	67.062	1.00 23.16	В
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•	MOTA	2474	CX	LEU	347	44.002	-7.790	67.561	1.00 23.19	В
	MOTA	2475	CB	LEU	347	44.678	-8.568	68.696	1.00 21.66	В
	MOTA	2476		LEU	347	45.955	-9.346	68.374	1.00 22.14	В
_	MOTA	2477	CD1	LEU	347	46.393	-10.118	69.613	1.00 20.42	В
5	MOTA	2478	CD2	LEU	347	45.718	-10.293	67.210	1.00 22.20	В
	MOTA	2479	С	LEU	347	42.679	-7.203	68.063	1.00 23.83	В
	MOTA	2480	0	LEU	347	41.617	-7.712	67.732	1.00 25.14	В
	MOTA	2481	N	SER	348	42.743	-6.135	68.854	1.00 21.92	В
	MOTA	2482	CA	SER	348	41.518	-5.530	69.368	1.00 23.12	В
10	ATOM	2483	CB	SER	348	41.839	-4.306	70.215	1.00 21.23	В
	MOTA	2484	· OG	SER	348	42.491	-4.707	71.402	1.00 27.13	В
	MOTA	2485	С	SER	348	40.582	-5.144	68.238	1.00 22.86	В
	MOTA	2486	0	SER	348	39.384	-5.348	68.331	1.00 22.12	В
	MOTA	2487	N	THR	349	41.156	-4.596	67.172	1.00 23.05	В
15	MOTA	2488	CA	THR	349	40.391	-4.186	66.005	1.00 25.38	В
	MOTA	2489	CB	THR	349	41.309	-3.483	64.988	1.00 25.69	В
	MOTA	2490	0G1	THR	349	41.656	-2.185	65.495	1.00 28.94	В
	MOTA	2491	CG2	THR	349	40.627	-3.334	63.639	1.00 26.37	В
	MOTA	2492	С	THR	349	39.714	-5.387	65.344	1.00 27.04	В
20	MOTA	2493	0	THR	349	38.502	-5.396	65.164	1.00 25.10	В
	MOTA	2494	N	LEU	350	40.505	-6.399	64.988	1.00 29.73	В
	MOTA	2495		LEU	350	39.971	-7.610	64.352	1.00 32.43	В.
	MOTA	2496	CB	LEU	350	41.112	-8.602	64.087	1.00 32.67	В
05	MOTA	2497		LEU	350	41.782	-8.523	62.709	1.00 33.86	. В
25	MOTA	2498	CD1		350	41.867	-7.089	62.243	1.00 35.72	В
	MOTA	2499	CD2		350	43.160	-9.140	62.777	1.00 34.30	В
	MOTA	250 0		LEU	350	38.880	-8.268	65.203	1.00 32.13	В
	MOTA	2501		LEU	350	37.869	-8.736	64.693	1.00 31.89	В
20	MOTA	2502		GLU	351	39.104	-8.286	66.510	1.00 32.99	В
30	MOTA	2503		GLU	351	38.163	-B.869	67.452	1.00 33.24	В
	MOTA	2504		GLU	351	38.807	-8.951	68.837	1.00 36.70	В
	MOTA	2505		GLU	351	38.014	-9.772	69.821	1.00 44.06	В
	MOTA	2506		GLU	351	37.791	-11.179	69.309	1.00 47.54	В
35 ⁻	MOTA	2507	0E1		351		-11.848	68.982	1.00 48.67	В
23	MOTA	2508	OE2		351	36.610	-11.599	69.228	1.00 48.07	8 B
•	ATOM	2509		GLU	351	36.901	-8.009 -8.532	67.519 67.584	1.00 31.83	B
	MOTA	2510 2511		GLU	351	35.778		67.503	1.00 32.33	В
	MOTA			TYR	352	37.097	-6.690 -5.727	67.550	1.00 25.10	В
40	MOTA	2512		TYR	352 352	35.997 36.561	-4.318	67.758	1.00 23.54	В
40	MOTA MOTA	2513 2514		TYR TYR	352	35.537	-3.220	67.970	1.00 23.52	В
	.ATOM	2515	CD1		352	34.862	-2.642	66.893	1.00 21.07	В
	ATOM	2516	CEI		352	33.952	-1.601	67.086	1.00 22.50	В
	ATOM	2517	CD2		352	35.271	-2.734	69.254	1.00 23.10	В
45	ATOM	2518	CE2		352	34.366	-1.699	69.464	1.00 22.61	В
	ATOM	2519		TYR	352	33.712	-1.134	68.377	1.00 25.05	В
	MOTA	2520		TYR	352	32.840	-0.085	68.577	1.00 29.15	B
	ATOM	2521		TYR	352	35.169	-5.790	66.262	1.00 23.04	В
	ATOM	2522		TYR	352	33.957	-5.819	66.309	1.00 21.96	В
50	MOTA	2523		ALA	353	35.841	-5.821	65.117	1.00 21.97	В
	MOTA	2524		ALA	353	35.155	-5.883	63.826	1.00 24.73	В
	ATOM	2525	СB	ALA	353	36.163	-5.732	62.692	1.00 21.20	В
	ATOM	2526	С	ALA	353	34.380	-7.192	63.663	1.00 26.52	В
	MOTA	2527	0	ALA	353	33.283	-7.210	63.119	1.00 25.94	В
55	ATOM	2528	N	HIS	354	34.978	-8.282	64.138	1.00 30.11	В
	ATOM	2529	CA	HIS	354	34.375	-9.607	64.052	1.00 32.42	В
	MOTA	2530	CB	HIS	354	35.334	-10.660	64.626	1.00 35.26	В
	MOTA	2531	CG	HIS	354	34.939	-12.073	64.317	1.00 38.11	В.
	ATOM	2532	CD2	HIS	354	34.416	-13.045	65.103	1.00 38.24	В
60	MOTA	2533	ND1	HIS	354	35.045	-12.614	63.053	1.00 39.29	В
	MOTA	2534	CE1	HIS	354		-13.858	63.072	1.00 38.94	В
	MOTA	2535	NE2	HIS	354		-14.143	64.303	1.00 39.79	В
	ATOM	2536		HIS	354	33.050	-9.642	64.811	1.00 33.09	В
	MOTA	2537		HIS	354		-10.127	64.297	1.00 33.51	В
65	MOTA	2538		ARG	355	33.053	-9.122	66.034	1.00 33.22	В
	MOTA	2539		ARG	355	31.847	-9.091	66.852	1.00 35.31	В
	MOTA	2540		ARG	355	32.145	-8.470	68.220	1.00 38.27	В
	MOTA	2541		ARG	355	32.976	-9.320	69.155	1.00 41.93	В
70	MOTA	2542		ARG	355	33.322	-8.539	70.416	1.00 44.68	В
70	MOTA	2543		ARG	355	32.132	-8.099	71.142	1.00 46.84	В
	MOTA	2544		ARG	355	31.299	-8.915	71.781	1.00 48.76	В
	MOTA	2545	NH1		355	31.523	-10.222	71.785	1.00 48.40	В
	ATOM	2546	NH2	AKG	355	30.243	-8.423	72.420	1.00 47.82	В

	MOTA	2547	С	ARG	355	30.740	-8.281	66.173	1.00 35.52	В
	MOTA	2548	0	ARG	355	29.564	-8.610	66.297	1.00 36.07	В
	ATOM	2549	N	ALA	356	31.124	-7.228	65.454	1.00 33.02	В
	MOTA	2550	ÇA	ALA	356	30.146	-6.374	64.789	1.00 31.19	В
5	ATOM	2551	СВ	ALA	356	30.837	-5.156	64.206	1.00 31.50	В
-	ATOM	2552	c	ALA	356	29.342	-7.089	63.704	1.00 31.06	В
		2553	ō	ALA	356	28.259	-6.645	63.343	1.00 28.55	В
	ATOM			LYS	357	29.880	-8.197	63.194	1.00 31.69	B
	MOTA	2554	N						1.00 33.26	В
10	MOTA	2555	CA	LYS	357		-8.973	62.144		
10	MOTA	2556	СВ	LYS	357		-10.198	61.768	1.00 35.45	В
	MOTA	2557	CG	LYS	357		-9.906	61.350	1.00 36.26	В
	MOTA	2558	යා	LYS	357	31.791	-10.458	59.956	1.00 39.94	В
	MOTA	2559	CE	LYS	357	31.524	-11.968	59.851	1.00 40.54	В
	MOTA	2560	NZ	LYS	357	32.455	-12.795	60.666	1.00 40.76	В
15	ATOM	2561	С	LYS	357	27.816	-9.447	62.552	1.00 33.43	В
~~	MOTA	2562	ō	LYS	357	26.911	-9.512	61.724	1.00 33.00	В
	ATOM	2563	N	ASN	358	27.654	-9.773	63.833	1.00 34.87	В
	ATOM			ASN	358		-10.253	64.379	1.00 36.60	В
		2564	CA				-10.942	65.724	1.00 37.20	В
20	ATOM	2565	CB	ASN	358					В
20	MOTA	2566	CG	ASN	358		-12.159	65.606	1.00 38.73	B
	MOTA	25€7		ASN	358		-12.602	66.589	1.00 40.28	
	ATOM	2568	ND2	ASN	358		-12.713	64.404	1.00 38.63	В
	ATOM	2569	С	ASN	358	25.320	-9.170	64.574	1.00 37.65	, В
	ATOM	2570	0	ASN	358	24.431	-9.322	65.406	1.00 38.18	В
25	ATOM	2571	N	ILE	359	25.413	-8.076	63.825	1.00 38.97	В
	ATOM	2572	CA	ILE	359	24.430	-7.003	63.951	1.00 40.85	В
	ATOM	2573	CB	ILE	359	25.088	-5.608	63.869	1.00 40.68	В
	ATOM	2574		ILE	359	24.014	-4.529	63.858	1.00 40.16	В
	ATOM	2575		ILE	359	26.019	-5.402	65.066	1.00 40.61	В
30	ATOM	2576		ILE	359	26.871	-4.161	64.970	1.00 39.58	В
50					359	23.391	-7.132	62.847	1.00 41.96	В
	MOTA	2577	C	ILE		23.391				В
	ATOM	2578	0		. 359		-7.227	61.671	1.00 42.22 1.00 43.88	В
	ATOM	2579	N	LEU	360.	22.122	-7.140	63.241		
25	MOTA	2580	CA	LEU	360	21.024	-7.276	62.293	1.00 46.61	В
35	MOTA	2581	CB	LEU	360	19.952	-8.212	62.864	1.00 48.74	В
	MOTA	2582	CG	LEU	360	19.660	-9.524	62.123	1.00 52.19	В
	MOTA	2583	CD1	LEU	360	18.886	-10.456	63.043	1.00 51.91	В
	MOTA	2584	CD2	LEU	360	18.870	-9.248	60.836	1.00 53.68	В
	MOTA	2585	С	LEU	360	20.406	-5.927	61.966	1.00 46.77	В
40	MOTA	2586	0	LEU	360	19.969	-5.211	62.854	1.00 46.72	B
	ATOM	2587	N	ASN	361	20.380	-5.586	60.681	1.00 47.32	В
	MOTA	2588	CA	ASN	361	19.805	-4.320	60.242	1.00 48.31	В
	MOTA	2589	CB	ASN	361	20.834	-3.502	59.458	1.00 47.61	В
	ATOM	2590	CG	ASN	361	21.795	-2.743	60.360	1.00 48.03	В
45		2591		ASN	361	22.423	-1.777	59.933	1.00 48.30	В
45	ATOM			ASN		21.913	-3.175	61.609	1.00 47.01	В
	ATOM	2592			361			59.387	1.00 49.65	В
	ATOM	2593	С	ASN	361	18.563	-4.526			В
	ATOM	2594	0	ASN	361	18.294	-5.627	58.919	1.00 51.43	В
50	MOTA	2595	N	LYS	362	17.821	-3.443	59.180	1.00 51.11	
50	MOTA	2596	CA	LYS	362	16.586	-3.452	58.400	1.00 50.99	В
	ATOM	2597	CB	LYS	362	16.883	-3.545	56.896	1.00 50.83	В
	MOTA	2598	CG	LYS	362	17.289	-2.229	56.253	1.00 49.23	В
	ATOM	2599	CD	LYS	362	17.117	-2.268	54.740	1.00 48.73	В
	ATOM	2600	CE	LYS	362	15.643	-2.244	54.329	1.00 47.35	В
55	MOTA	2601	NŽ	LYS	362	14.989	-0.914	54.515	1.00 44.68	В
	MOTA	2602	C	LYS	362	15.659	-4.588	58.814	1.00 51.66	В
	MOTA	2603	ŏ	LYS	362	15.211	-5.329	57.913	1.00 52.28	В
	ATOM	2604		LYS	362	15.387	-4.712	60.031	1.00 50.87	В
							10.621	59.419	1.00 27.37	-
60	MOTA	2605	MG	MG	2602	43.651				ADP
OU	ATOM	2606	PB	ADP	2600	44.241	7.165	60.136	1.00 25.05	
	MOTA	2607		ADP		44.666	7.765	61.419	1.00 26.27	ADP
	MOTA	2608		ADP	2600	43.842	5.630	60.325	1.00 30.28	ADP
	ATOM	2609		ADP	2600	43.097	7.920	59.552	1.00 28.27	ADP
	MOTA	2610	PA	ADP	2600	45.608	7.818	57.697	1.00 39.43	ADP
65	ATOM	2611	Ola	ADP	2600	44.613	7.286	56.772	1.00 38.84	ADP
	MOTA	2612		ADP	2600	45.462	9.276	57.778	1.00 41.49	ADP
	MOTA	2613		ADP	2600	45.426	7.167	59.121	1.00 32.30	ADP
	ATOM	2614		ADP	2600	47.084	7.550	57.187	1.00 39.41	ADP
	MOTA	2615		ADP	2600	48.157	6.858	57.828	1.00 42.82	ADP
70	MOTA	2616		ADP	2600	49.374	6.940	56.825	1.00 45.97	ADP
, 0				ADP		49.399	5.696	56.137	1.00 46.62	ADP
	MOTA	2617			2600					ADP
	MOTA	2618		ADP	2600	49.266	8.021	55.715	1.00 46.20	
	MOTA	2619	03*	ADP	2600	50.512	8.717	55.502	1.00 49.03	ADP

	MOTA	2620	C2*	ADP	2600	48.810	7.296	54.462	1.00 46.75	ADP
	MOTA	2621	02*	ADP	2600	49.235	7.921	53.240	1.00 48.13	ADP
	ATOM	2622	C1 *	ADP	2600	49.328	5.886	54.701	1.00 47.35	ADP
	MOTA	2623	N9	ADP	2600	48.435	4.815	54.144	1.00 48.03	ADP
5	MOTA	2624	C8	ADP	2600	47.417	4.221	54.811	1.00 47.72	ADP
,										
	ATOM	2625	N7	ADP	2600	46.839	3.328	54.046	1.00 48.56	ADP
	MOTA	2626	C5	ADP	2600	47.454	3.316	52.892	1.00 49.10	ADP
	ATOM	2627	C6	ADP	2600	47.308	2.603	51.707	1.00 49.07	ADP
	MOTA	2628	N6	ADP	2600	46.350	1.680	51.610	1.00 49.43	ADP
10	MOTA	2629	N1	ADP	2600	48.159	2.844	50.628	1.00 50.04	ADP
10	ATOM	2630	C2	ADP	2600	49.152	3.776	50.684	1.00 48.98	ADP
									1.00 50.49	ADP
	ATOM	2631	N3	ADP	2600	49.301	4.478	51.842		
	ATOM	2632	C4	ADP	2600 -	48.491	4.283	52.944	1.00 48.96	ADP
	MOTA	2633	C1	2-7	1	37.376	16.487	53.441	1.00 31.12	2-7
15	ATOM	2634	C2	2-7	1	38.554	16.442	52.639	1.00 31.01	2-7
	MOTA	2635	C3	2-7	1	38.554	15.433	51.622	1.00 31.01	2-7
	MOTA	2636	C4	2-7	1	37.388	14.559	51.530	1.00 29.91	2-7
	ATOM	2637	Ç5	2-7	ī	36.248	14.570	52.396	1.00 29.25	2-7
			C6	2-7	î	36.296	15.546	53.415	1.00 30.61	2-7
20	MOTA	2638								2-7
20	ATOM	2639		2-7	1	39.708	15.357	50.686	1.00 30.99	
	MOTA	2640		2-7	1	40.272	16.598	50.056	1.00 33.35	2-7
	MOTA	2641	N12	2-7	1	41.446	16.158	49.317	1.00 33.73	2-7
	MOTA	2642	C13	2-7	1	41.189	14.730	49.013	1.00 31.60	2-7
	ATOM	2643		2-7	1	40.419	14.175	50.202	1.00 30.03	2-7
25	ATOM	2644		2-7	1	41.032	14.136	47.645	1.00 28.72	2-7
23		2645		2-7	î	42.014	13.131	47.164	1.00 27.73	2-7
	MOTA								1.00 26.29	2-7
	MOTA	2646		2-7	1	41.952	12.752	45.765		
	ATOM	2647		2-7	1	40.984	13.380	44.878	1.00 26.40	2-7
00	MOTA	2648		2-7	1	39.931	14.256	45.351	1.00 27.79	2-7
30	MOTA	2649	C23	2-7	1	39.958	14.694	46.762	1.00 27.64	2-7
	ATOM	2650	C29	2-7	1	42.438	17.110	49.102	1.00 34.81	2-7
	MOTA	2651		2-7	1	43.717	16.767	49.283	1.00 35.06	2~7
	ATOM	2652		2-7	ī	44.603	17.929	49.086	1.00 31.67	2-7
	ATOM	2653		2-7	î	44.177	15.446	49.734	1.00 32.58	2-7
35										2-7
22	ATOM	.2654		2-7	1	42.187	18.279	48.762	1.00 35.09	
	MOTA	2655		2-7	1	37.369	13.692	50.535	1.00 32.42	2-7
	ATOM	2656	F41	2-7	1	37.291	17.497	54.277	1.00 33.09	2-7
	MOTA	2657	0	нон	2	38.630	10.603	62.535	1.00 3.96	S
	MOTA	2658	0	нон	3	28.064	20.853	56.798	1.00 15.26	s
40	ATOM	2659	o	нон	4	43.423	-1.052	63.682	1.00 6.84	S
	ATOM	2660	ŏ	нон	5	41.471	9.650	60.748	1.00 28.56	s
					6			61.146	1.00 22.21	s
	MOTA	2661	0	нон		53.043				s
	MOTA	2662	0	нон	8	43.351	23.546	43.947	1.00 14-88	
4.5	MOTA	2663	0	нон	11	31.538	6.420	79.791	1.00 20.07	s
45	MOTA	2664	0	HOH	12	44.364	1.570	53.833	1.00 33.76	S
	ATOM	2665	0	HOH	13	42.141	-0.803	71.483	1.00 23.37	s
	MOTA	2666	0	нон	17	50.048	-0.508	68.644	1.00 38.33	s
	ATOM	2667	Ó	нон	18	42.525	8.183	64.075	1.00 31.71	s
	ATOM	2668	ŏ	нон	20	49.961	-5.304	63.635	1.00 28.76	s
50			ŏ			52.974	11.228	41.771	1.00 27.37	s
50	MOTA	2669		нон	21					S
	MOTA	2670	0	нон	23	44.880	17.208	64.490	1.00 19.87	
	MOTA	2671	0	нон	25	33.865	11.390	57.228	1.00 14.50	s
	MOTA	2672	0	нон	26	42.746	19.345	56.865	1.00 19.80	s
	MOTA	2673	0	нон	27	43.217	3.216	42.636	1.00 29.84	S
55	MOTA	2674	0	нон	28	47.542	18.783	69.096	1.00 24.56	S
	MOTA	2675	ō	нон	29	29.606	-8.997	58.639	1.00 41.51	. S
	MOTA	2676	ŏ	нон	30	38.143	15.249	61.346	1.00 12.36	s
										s
	MOTA	2677	0	нон	31	47.769	14.311	41.568	1.00 24.48	
60	MOTA	2678	0	нон	32	22.227	19.477	42.995	1.00 35.68	S
60	MOTA	2679	0	нон	34	38.077	4.715	80.434	1.00 19.14	s
	ATOM	2680	0	нон	35	27.208	25.794	60.457	1.00 30.49	s
	ATOM	2681	0	нон	40	45.874	21.711	68.966	1.00 14.93	S
	ATOM	2682	ō	нон	42	37.931	3.241	64.945	1.00 21.80	s
		2683						71.900	1.00 38.67	s
65	MOTA		0	HOH	44	33.173	12.293			s
UJ	MOTA	2684	0	нон	45	38.986	3.636	49.470	1.00 20.20	
	MOTA	2685	0	нон	46	35.162	19.890	41.213	1.00 25.42	S
	MOTA	2686	0	нон	52	22.755	-3.615	56.949	1.00 33.63	S
	MOTA	2687	0	нон	53	27.917	6.206	79.432	1.00 19.49	s
	MOTA	2688	0	нон	55	37.862	4.182	47.024	1.00 13.89	S
70	MOTA	2689	ō	нон	57	31.462	4.272	82.519		s
, ,	ATOM	2690					12.586	58.140	1.00 18.34	s
			0	нон	59	38.826				
	MOTA	2691	0	нон	60	27.879	4.380		1.00 24.90	S
	MOTA	2692	0	нон	61	45.041	10.037	53.740	1.00 42.66	S

	ATOM	2693	0	нон	62	28.763	26.533	62.454	1.00 35.09	s
	ATOM	2694	ō	нон	66	38.448	-0.512	37.739	1.00 44.71	S
	ATOM	2695	ŏ	нон	67	31.394	24.733	63.775	1.00 40.50	S
	ATOM	2696	ŏ	нон	68	40.487	5.787	72.041	1.00 37.21	s
5	ATOM	2697	ŏ	нон	69	52.548	19.976	38.009	1.00 24.27	S
_	ATOM	2698	ō	нон	70	40.043	-1.641	68.804	1.00 21.10	s
	ATOM	2699	ō	нон	71	21.370	18.117	39.097	1.00 47.89	s
	ATOM	2700	ŏ	нон	73	45.431	-1.388	51.309	1.00 36.21	S
	ATOM	2701	ō	нон	74	12.109	0.216	54.870	1.00 45.32	s s
10	ATOM	2702	ŏ	нон	78	41.390	5.467	40.236	1.00 31.36	s
10	ATOM	2703	ŏ	нон	79	38.398		49.709	1.00 28.25	S
	ATOM	2704	ŏ	нон	84	46.457	-1.971	63.989	1.00 20.69	S
	ATOM	2705	ŏ	нон	87	2.291	6.433	36.064	1.00 27.27	S
	ATOM	2706	ŏ	нон	88	46.187	3.359	74.292	1.00 30.60	S
15	ATOM	2707	ŏ	нон	89	51.911	4.577	56.634	1.00 44.94	S
	ATOM	2708	ŏ	нон	90	45.811	18.580	66.703	1.00 26.87	s
	ATOM	2709	ō	нон	91	47.734	13.013	72.702	1.00 32.94	s
	MOTA	2710	ŏ	нон	92	23.555	15.386	53.064	1.00 29.56	S
	ATOM	2711	ŏ	нон	93	43.670	-2.643	73.172	1.00 27.18	s
20	ATOM	2712	ŏ	нон	94	27.978	20.947	70.487	1.00 41.48	s
	ATOM	2713	ō	нон	95	44.678	-7.04B	71.862	1.00 24.48	s
	ATOM	2714	ō	нон	97	37.124	2.776	73.009	1.00 36.39	S
	ATOM	2715	ō	нон	98	32.730	25.500	47.607	1.00 42.43	S
	MOTA	2716	ō	нон	101	46.793	22.739	62.116	1.00 28.62	S
25	MOTA	2717	0	нон	104	20.079	21.304	46.635	1.00 44.83	S
	ATOM	2718	0	нон	105	30.653	-3.670	75.744	1.00 35.11	s
	ATOM	2719	٥	нон	106	46.987	13.182	34.815	1.00 16.99	S
	ATOM	2720	0	нон	109	43.794	0.066	55.803	1.00 30.02	s s
	ATOM	2721	0	HOH	111	25.208	9.102	28.662	1.00 32.86	s
30	ATOM	2722	0	нон	113	44.655	15.401	59.741	1.00 25.68	s
	ATOM	2723	0	HOH	115	18.285	12.456	33.587	1.00 30.40	s s
	MOTA	2724	0	нон	116	47.999	-0.217	48.915	1.00 36.92	S
	MOTA	2725	0	HOH	117	23.508	25.313	66.864	1.00 47.95	S
0.5	MOTA	2726	0	нон	119		-14.904	55.904	1.00 35.41	s
35	ATOM	2727	О	нон	120	47.343	8.255	68.520	1.00 37.89	s
	MOTA	2728	0	HOH	128	28.608	-6.298	48.882	1.00 26.00	S
	MOTA	2729	0	HOH	132	6.107	15.208	42.672	1.00 30.09	s
	ATOM	2730	0	HOH	133	26.812	14.766	57.900	1.00 17.88	S
in	ATOM	2731	0	HOH	135	46.950	10.746	67.779	1.00 31.59	S
40	MOTA	2732	0	нон	136	24.332	1.606	79.565	1.00 28.86	s s
	MOTA	2733	0	нон	138	50.215	2.473	62.680	1.00 35.95	S
	MOTA	2734	0	нон	139	22.069	24.748	54.683	1.00 25.56	s
	ATOM	2735	0	нон	140		-18.491	58.486	1.00 49.65	s
15	MOTA	2736	0	нон	141	15.900	-4.594	62.687	1.00 33.93	s
45	MOTA	2737	0	нон	143	14.793	-3.866	47.507	1.00 45.81	S

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TABLE 4

	REMARK	FILEN	AME=	Comp	ound 4	-2a_2dpb.pdl	o *				
_	!CRYST	69	. 200	79	.400	159.200 90.			P21212		
5	ATOM	2605	CB	LYS	17		-12.132	60.197	1.00 9		В
	MOTA	2606	CC	LYS	17		-12.714	59.720		53.46	В
	ATOM	2607	CD	LYS	17		-12.276	58.298	1.00 9		В
	ATOM	2608	CE	LYS	17		-13.129	57.240	1.00		В
10	MOTA	2609	NZ	LYS	17	24.977	-13.074	57.341	1.00 9		В
10	MOTA	2610	C	LYS	17	24.464	-9.793	59.322	1.00 4		В
	MOTA	2611	0	LYS	17	25.371	-9.870	58.525	1.00 4		В
	MOTA	2612	N	LYS	17	23.273	-10.326	61.434	1.00		В
	ATOM	2613	CA	LYS	17		-10.640	60.578	1.00 4		B B
15	ATOM	2614	N	ASN	18	23.441 23.346	-8.969 -8.128	59.167 57.990	1.00		B
IJ	ATOM ATOM	2615 2616	CA	ASN ASN	18 18	22.016	-7.375	58.014	1.00		В
	MOTA	2617	CG	ASN	18	21.059	-7.856	56.934		45.64	В
	MOTA	2618		ASN	18	21.222	-7.538	55.748	1.00		В
	MOTA	2619		ASN	18	20.068	-8.642	57.331	1.00		B
20	MOTA	2620	C	ASN	18	24.508	-7.150	57.750	1.00		В
	ATOM	2621	0	ASN	18	24.895	-6.921	56.596	1.00		В.
	ATOM	2622	N	ILE	19	25.077	-6.584	58.810	1.00	36.30	- B
	MOTA	2623	CA	ILE	19	26.171	-5.618	58.668	1.00	32.31	В
~ ~	ATOM	2624	CB	ILE	19	26.495	-4.982	60.043	1.00	33.05	В
25	ATOM	2625		ILE	19	26.959	-6.042	61.012	1.00		В
	ATOM	2626		ILE	19	27.599	-3.938	59.905	1.00		В
	MOTA	2627		ILE	19	27.845	-3.169	61.165	1.00		В
	MOTA	2628	С	ILE	19	27.464	-6.184	58.058	1.00		В
30	MOTA	2629	0	ILE	19	28.021	-7.161	58.574	1.00		В
30	MOTA	2630	N	GLN	20	27.934	-5.566	56.967	1.00		
	MOTA	2631	CY	GLN	20	29.174	-5.986	56.285	1.00		B B
	MOTA	2632	CB	GLN GLN	20 20	29.216 30.526	-5.493 -5.834	54.839 54.127	1.00		B
	MOTA NOTA	.2633 2634	CG CD	GLN	20	30.589	-5.290	52.715	1.00		В
35	MOTA	2635		GLN	20	30.540	-4.089	52.514	1.00		В
JJ	MOTA	2636		GLN	20	30.720	-6.173	51.737	1.00		В
	ATOM	2637	c	GLN	20	30.450	-5.437	56.952	1.00		В
	ATOM	2638	ŏ	GLN	20	30.566	-4.239	57.180	1.00		В
	ATOM	2639	N	VAL	21	31.394	-6.328	57.254	1.00	9.34	В
40	MOTA	2640	CA	VAL	21	32.656	-5.941	57.880	1.00	6.24	В
	MOTA	2641	CB	VAL	21	32.775	-6.537	59.296	1.00	5.92	В
	MOTA	2642		VAL	21	34.094	-6.144	59.934	1.00	3.44	В
	ATOM	2643	CG2	VAL	21	31.616	-6.056	60.138	1.00	7.73	В
45	MOTA	2644	С	VAL	21	33.868	-6.396	57.052	1.00	5.09	В
45	ATOM	2645	0	VAL	21	34.031	-7.569		.1.00	4.24	В
	MOTA	2646	N	VAL	22	34.715	-5.454	56.659	1.00	3.75	В
	MOTA	2647	CA	VAL	22	35.893	-5.805	55.879	1.00	4.12	B B
	MOTA MOTA	2648 2649	CB	VAL VAL	22 22	35.819 34.566	-5.226 -5.731	54.420 53.703	1.00	3.36 3.16	В
50	ATOM	2650		VAL	22	35.823	-3.717	54.452	1.00	2.87	В
50	ATOM	2651	C	VAL	22	37.157	-5.305	56.553	1.00	6.20	В
	ATOM	2652	õ	VAL	22	37.122	-4.365	57.352	1.00	6.79	В
	MOTA	2653	Ň	VAL	23	38.271	-5.946	56.223	1.00	4.46	В
	ATOM	2654	CA	VAL	23	39.559	-5.585	56.785	1.00	4.23	В
55	ATOM	2655	CB	VAL	23	40.195	-6.830	57.477	1.00	4.02	В
	ATOM	2656	CG1	VAL	23	41.555	-6.511	58.081	1.00	1.86	В.
	ATOM	2657	CG2	VAL	23	39.268	-7.319	58.550	1.00	5.77	В
	ATOM	2658	С	VAL	23	40.505	-5.037	55.710	1.00	4.46	B
	ATOM	2659	0	VAL	23	40.553	-5.531	54.586	1.00	4.66	В
60	ATOM	2660	N	ARG	24	41.251	-3.998		1.00	7.29	В
	MOTA	2661	CA	ARG	24	42.228	-3.436	55.128	1.00	9.87	В
	MOTA	2662	CB	ARG	24	41.793	-2.092	54.531	1.00	6.53	В
	MOTA	2663	CG	ARG	24	42.744	-1.662		1.00	6.89	В
65	MOTA	2664	CD	ARG	24	42.401	-0.306	52.837	1.00	7.91	В
65	MOTA	2665	NE	ARG	24	43.142	-0.040		1.00	4.86	В
	MOTA	2666	CZ	ARG	24	43.041	1.095	50.909	1.00	3.46	В
	MOTA	2667		ARG	24	42.228	2.056	51.329	1.00	1.00	B B
	ATOM ATOM	2668 2669	C NHZ	ARG ARG	24 24	43.773 43.541	1.287 -3.179	49.814 55.856	1.00	1.00	B
70	ATOM	2670	0	ARG	24	43.586	-2.374	56.791	1.00		В
, 0	ATOM	2671	N	CYS	25	44.593	-3.873		1.00		В

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	ATOM	2672	CA	CYS	25	45.928	-3.742	55.996	1.00 16.78	В
	ATOM	2673	CB	CYS	25	46.646	-5.088	55.932	1.00 14.53	В
	MOTA	2674	SG	CYS	25	48.149	-5.147	56.865	1.00 15.92	В
										В
5	MOTA	2675	С	CYS	25	46.743	-2.706	55.216	1.00 17.93	
)	ATOM	2676	0	CYS	25	46.793	-2.743	53.991	1.00 19.83	В
	MOTA	2677	N	ARG	26	47.369	-1.774	55.922	1.00 20.13	В
	MOTA	2678	CA	ARG	26	48.186	-0.779	55.242	1.00 23.56	В
	MOTA	2679	CB	ARG	26	48.410		56.122	1.00 23.04	В
							0.441			
10	MOTA	2680	CG	ARG	26	49.018	0.108	57.480	1.00 25.34	В
10	MOTA	2681	CD	ARG	26	49.478	1.335	58.248	1.00 25.85	В
	MOTA	2682	NE	ARG	26	50.882	1.635	57.970	1.00 27.66	В
					26			58.830	1.00 29.35	В
	ATOM	2683	CZ	ARG		51.876	1.425			
	MOTA	2684		ARG	26	51.620	0.914	60.030	1.00 28.00	В
	MOTA	2685	NH2	ARG	26	53.126	1.729	58.494	1.00 29.65	В
15	MOTA	2686	C	ARG	26	49.566	-1.360	54.924	1.00 26.17	В
	ATOM	2687	ŏ	ARG	26	49.965	-2.367	55.500	1.00 27.47	В
	MOTA	2688	N	PRO	27	50.296	-0.748	53.976	1.00 28.46	В
	MOTA -	2689	CΩ	PRO	27	49.815	0.221	52.972	1.00 28.96	В
	ATOM	2690	CA	PRO	27	51.634	-1.225	53.617	1.00 30.05	В
20	ATOM	2691	CB	PRO	27	51.757	-0.791	52.157	1.00 29.21	В
LU										
	MOTA	2692	CG	PRO	27	51.081	0.508	52.153	1.00 27.78	В
	ATOM	2693	С	PRO	27	52.652	-0.565	54.551	1.00 30.74	В
	ATOM	2694	0	PRO	27	52.315	0.387	55.255	1.00 30.33	В
	MOTA	2695	N	PHE	28	53.888	-1.065	54.559	1.00 33.00	В
25										
23	ATOM	2696	CA	PHE	28	54.946	-0.488	55.397	1.00 35.47	В
	MOTA	2697	CB	PHE	28	56.197	-1.349	55.423	1.00 34.78	В
	ATOM	2698	CG ·	PHE	28	56.043	-2.621	56.180	1.00 34.30	В
	MOTA	2699		PHE	28	55.970	-3.848	55.506	1.00 33.11	В
20	ATOM	2700		PHE	28	55.975	-2.598	57.566	1.00 34.50	В
30	MOTA	2701	CE1	PHE	28	55.831	-5.030	56.204	1.00 32.04	B
	MOTA	2702	CE2	PHE	28	55.833	-3.779	58.283	1.00 34.83	В
	MOTA	2703	CZ	PHE	28	55.762	-5.002	57.594	1.00 34.76	В
	MOTA	2704	С	PHE	28	55.432	0.848	54.837	1.00 37.44	В
~ -	ATOM	2705	0	PHE	28	55.529	1.019	53.640	1.00 37.96	В
35	MOTA	2706	N	ASN	29	55.724	1.797	55.719	1.00 41.21	В
	ATOM	2707	CA	ASN	29	56.195	3.114	55.288	1.00 43.97	В
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	ATOM	2708	CB	ASN	29	55.731	4.190	56.280	1.00 42.30	В
	MOTA	2709	CG	ASN	29	56.080	3.843	57.724	1.00 41.84	В
	ATOM	2710	OD1	ASN	29	57.230	3.554	58.038	1.00 40.87	В
40	ATOM	2711		ASN	29	55.080	3.866	58.604	1.00 40.16	В
										В
	ATOM	2712	С	ASN	29	57.718	3.112	55.190	1.00 47.03	
	MOTA	2713	0	ASN	29	58.361	2.179	55.651	1.00 48.57	В
	ATOM	2714	N	LEU	30	58.290	4.156	54.594	1.00 49.85	В
	MOTA	2715	CA	LEU	30	59.745	4.258	54.442	1.00 52.56	В
45	MOTA	2716	CB	LEU	30	60.125	5.641	53.928	1.00 52.63	В
73										
	MOTA	2717	CC	LEU	30	60.214	5.735	52.409	1.00 53.20	В
	MOTA	2718	CD1	LEU	30	60.395	7.194	51.973	1.00 53.18	В
	ATOM	2719	CD2	LEU	30	61.378	4.862	51.935	1.00 54.30	В
	ATOM	2720	С	LEU	30	60.579	3.978	55.695	1.00 54.36	В
50										
50	ATOM	2721	0	LEU	30	61.623	3.347	55.619	1.00 54.97	В
	MOTA	2722	N	ALA	31	60.121	4.453	56.847	1.00 56.36	В
	MOTA	2723	CA	ALA	31	60.843	4.228	58.097	1.00 58.76	В
	MOTA	2724	CB	ALA	31	60.214	5.057	59.202	1.00 58.55	В
	ATOM	2725	c	ALA	31	60.842	2.742	58.487	1.00 60.40	В
55										
JJ	MOTA	2726	0	ALA	31	61.749	2.266	59.167	1.00 60.67	В
	MOTA	2727	N	GLU	32	59.819	2.016	58.045	1.00 61.95	В
	ATOM	2728	CA	GLU	32	59.692	0.594	58.350	1.00 63.39	В
	MOTA	2729	СВ	GLU	32	58.215	0.187	58.322	1.00 62.91	В
		2730								В
40	MOTA		CG	GLU	32	57.429	0.683	59.524	1.00 62.16	
60	ATOM	2731	CD	GLU	32	55.933	0.669	59.299	1.00 61.37	В
	ATOM	2732	OE1	GLU	32	55.191	0.841	60.289	1.00 60.97	В
	MOTA	2733		GLU	32	55.504	0.497	58.138	1.00 60.36	В
	MOTA	2734	С	GLU	32	60.487	-0.318	57.414	1.00 64.76	В
	MOTA	2735	0	GLU	32	61.130	-1.261	57.860	1.00 64.21	B
65	MOTA	2736	N	ARG	33	60.436	-0.039	56.116	1.00 66.90	В
	MOTA	2737	CA	ARG	33	61.150	-0.855	55.141	1.00 69.19	В
	MOTA	2738	СВ	ARG	33	60.690	-0.503	53.719	1.00 70.74	В
	MOTA	2739	CG	ARG	33	60.911	0.953	53.310	1.00 73.78	В
	ATOM	2740	CD	ARG	33	60.238	1.267	51.977	1.00 75.17	В
70	ATOM	2741	NE	ARG	33	60.663	0.349	50.920	1.00 76.52	В
, 0										
	MOTA	2742	CZ	ARG	33	61.889	0.301	50.400	1.00 76.92	В
	MOTA	2743	NH1	ARG	33	62.838	1.122	50.829	1.00 76.57	В
	ATOM	2744	NH2		33	62.168	-0.569	49.441	1.00 78.04	В
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	ATOM	2745	c	ARG	33	62.650	-0.654	55.297	1.00 70.11	В
	MOTA	2746	0	ARG	33	63.439	-1.524	54.943	1.00 70.36	B B
	MOTA	2747	N	LYS	34	63.038	0.500	55.832	1.00 71.13	В
5	MOTA	2748	CA	LYS	34	64.447	0.798 2.254	56.053 56.498	1.00 73.21	В
,	ATOM ATOM	2749 2750	CB CG	LYS LYS	34 34	64.623 64.611	3.267	55.363	1.00 74.27	В
	MOTA	2751	CD	LYS	34	66.023	3.637	54.921	1.00 74.99	В
	MOTA	2752	CE	LYS	34	66.769	2.463	54.306	1.00 74.88	В
	MOTA	2753	NZ	LYS	34	68.154	2.852	53.916	1.00 75.81	В
10	MOTA	2754	c	LYS	34	65.006	-0.137	57.123	1.00 72.12	В
	MOTA	2755	0	LYS	34	66.207	-0.424	57.142	1.00 72.82	В
	ATOM	2756	N	ALA	35	64.130	-0.612	58.007	1.00 71.37	В
	ATOM	2757	CA	ALA	35	64.522	-1.526	59.077	1.00 69.94	В
1.5	MOTA	2758	CB	ALA	35	63.780	-1.177	60.361	1.00 69.77	В
15	MOTA	2759	C	ALA	35	64.223	-2.970	58.685	1.00 69.24 1.00 69.32	B B
	MOTA	2760	0	ALA	35 36	64.198 64.001	-3.854 -3.194	59.542 57.388	1.00 69.32	В
	MOTA MOTA	2761 2762	N CA	SER SER	36	63.689	-4.519	56.848	1.00 66.99	В
	MOTA	2763	CB	SER	36	64.937	-5.405	56.860	1.00 67.27	В
20	ATOM	2764	OG	SER	36	65.906	-4.912	55.959	1.00 67.40	В
	MOTA	2765	¢	SER	36	62.579	-5.159	57.674	1.00 65.70	В
	ATOM	2766	Ó	SER	36	62.721	-6.270	58.185	1.00 65.65	₿.
	MOTA	2767	N	ALA	37	61.469	-4.435	57.791	1.00 64.41	В
0.5	ATOM	2768	CA	ALA	37	60.320	-4.880	58.568	1.00 62.00	В
25	MOTA	2769	CB	ALA	37	59.256	-3.784	58.601	1.00 62.35	В
	MOTA	2770	C	ALA	37	59.699	-6.185	58.093	1.00 59.79 1.00 58.90	B B
	MOTA	2771	0	ALA	37	59.490 59.400	-6.404 -7.042	56.909 59.061	1.00 58.30	В
	MOTA MOTA	2772 2773	N CA	HIS	38 38	58.795	-8.347	58.828	1.00 55.57	В
30	MOTA	2774	CB	HIS	38	59.420	-9.381	59.785	1.00 57.59	В
50	ATOM	2775	CG	HIS	38	59.426	-8.963	61.233	1.00 58.97	B
	ATOM	2776		HIS	38	58.878	-9.543	62.328	1.00 58.78	В
	MOTA	2777		HIS	38	60.083	-7.837	61.689	1.00 58.86	В
	MOTA	2778	CE1	HIS	38	59.939	-7.744	63.000	1.00 58.84	В
.35	MOTA	. 2779		HIS	38	59.211	-8.766	63.412	1.00 58.91	В
	MOTA	2780	C	HIS	38	57.296	-8.223	59.086	1.00 53.05	В
	MOTA	2781	0	HIS	38	56.890	-7.787	60.163	1.00 54.10	B B
	MOTA	2782	N	SER	39	56.472	-8.605 -8.500	58.114 58.290	1.00 48.25	В
40	MOTA MOTA	2783 2784	CA CB	SER SER	39 39	55.026 54.295	-8.575	56.970	1.00 42.55	В
40	MOTA	2785	OG	SER	39	52.903	-8.490	57.201	1.00 39.13	В
	ATOM	2786	c	SER	39	54.444	-9.616	59.130	1.00 40.52	В
	MOTA	2787	ō	SER	39	54.750	-10.773	58.919	1.00 39.58	В
	MOTA	2788	N	ILE	40	53.603	-9.247	60.092	1.00 38.79	В
45	MOTA	2789	CA	ILE	40	52.967	-10.222	60.979	1.00 36.32	В
	MOTA	2790	CB	ILE	40	53.039	-9.786	62.478	1.00 37.00	В
	MOTA	2791		ILE	40	54.493	-9.677	62.925	1.00 37.72	B B
	MOTA	2792		ILE	40	52.307	-8.458	62.692	1.00 37.68	В
50	MOTA	2793 2794		ILE	40 40	52.102 51.501	-8.097 -10.426	64.161 60.611	1.00 34.00	В
50	MOTA	2795	C 0	ILE	40	50.757	-11.084	61.319	1.00 32.93	В
	ATOM	2796	N	VAL	41 .	51.097	-9.863	59.482	1.00 33.39	В
	ATOM	2797	ĊA	VAL	41	49.720	-9.986	59.028	1.00 32.21	В
	MOTA	2798	СВ	VAL	41	48.982	-8.617	59.042	1.00 31.99	В
55	MOTA	2799		VAL	41	47.559	-8.778	58.536	1.00 30.52	В
	MOTA	2800	CG2	VAL	41	48.964	-8.048	60.445	1.00 32.73	В
	MOTA	2801	С	VAL	41	49.685	-10.526	57.610	1.00 32.35	В
	MOTA	2802	0	VAL	41	50.357	-10.022	56.728	1.00 31.91	В
۲۸	MOTA	2803	N	GLU	42		~11.565	57.417	1.00 33.52	B B
60	MOTA	2804	CA	GLU	42		-12.189	56.112	1.00 34.79	В
	MOTA	2805	CB	GLU	42		-13.626 -13.762	56.142 55.882	1.00 34.88	В
	MOTA	2806 2807	CD	GLU	42 42		-15.139	56.222	1.00 36.62	В
	MOTA	2808		GLU	42		-16.105	55.996	1.00 35.55	В
65	ATOM	2809		GLU	42		-15.262	56.704	1.00 36.67	B
	ATOM	2810	C	GLU	42		-12.207	55.689	1.00 34.67	В
	ATOM	2811	ō	GLU	42		-12.745	56.388	1.00 35.11	В
	MOTA	2812	N	CYS	43		-11.615	54.540	1.00 33.53	В
70	MOTA	2813	CA	CYS	43		-11.575	54.074	1.00 33.64	В
70	MOTA	2814	CB	CYS	43		-10.172	53.575	1.00 31.73	В
	ATOM	2815	SG	CYS	43	45.291	-8.913	54.863	1.00 30.24	В
	MOTA	2816	C	CYS	43		-12.597	52.985	1.00 34.68	B B
	MOTA	2817	0	CYS	43	46.052	-12.722	52.025	1.00 35.47	ь

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	ATOM	2818	N	ASP	44	44.220 - 43.821 -		53.160 52.196	1.00 34.51	B B
	ATOM ATOM	2819 2820	CA CB	ASP	44 44	43.698 -		52.196	1.00 37.74	В
	ATOM	2821	CC	ASP	44	43.627 -		51.880	1.00 39.14	В
5	ATOM	2822		ASP	44	43.029 -		50.787	1.00 38.15	В
_	ATOM	2823		ASP	44	44.166 -		52.206	1.00 40.23	В
	MOTA	2824	С	ASP	44	42.452 -	13.949	51.662	1.00 36.02	В
	MOTA	2825	0	ASP	44	41.433 -		52.228	1.00 34.41	В
••	MOTA	2826	N	PRO	45	42.415 -		50.566	1.00 36.48	В
10	ATOM	2827	CD	PRO	45	43.558 -		49.725	1.00 37.08	В
	MOTA	2828	CA	PRO	45	41.162 - 41.646 -		49.962 48.828	1.00 36.44	B B
	ATOM ATOM	2829 2830	CB CG	PRO PRO	45 45	42.892 -		48.398	1.00 37.61	В
	ATOM	2831	c	PRO	45		13.872	49.518	1.00 36.95	В
15	ATOM	2832	ō	PRO	45		13.805	49.685	1.00 37.27	В
	MOTA	2833	N	VAL	46	40.834 -	14.912	48.930	1.00 37.39	В
	ATOM	2834	CA	VAL	46	40.051 -	16.057	48.479	1.00 37.62	В
•	MOTA	2835	CB	VAL	46		17.087	47.773	1.00 38.49	В
20	MOTA	2836		VAL	46		18.269	47.334	1.00 39.31	В
20	MOTA	2837		VAL	46	41.642 -		46.584 49.665	1.00 38.33	B B
	ATOM ATOM	2838	C O	VAL VAL	46 46		16.728 17.082	49.606	1.00 38.03	В
	ATOM	2839 2840	N	ARG	47		16.902	50.752	1.00 37.10	В
	ATOM	2841	CA	ARG	47	39.520 -		51.947	1.00 37.76	В
25	MOTA	2842	CВ	ARG	47	40.627 -		52.797	1.00 40.98	В
	ATOM	2843	CG	ARG	47	40.138 -	19.170	53.811	1.00 45.53	В
	MOTA	2844	CD	ARG	47	40.088 -		53.205	1.00 48.08	В
	MOTA	2845	NE	ARG	47	41.427 -		52.905	1.00 51.05	В
30	MOTA	2846	CZ	ARG	47 47	42.361 - 42.101 -		53.826 55.108	1.00 53.04	B B
50	MOTA MOTA	2847 2848		ARG ARG	47	43.558 -		53.467	1.00 53.55	В
	ATOM	2849	C	ARG	47	38.817 -		52.774	1.00 35.87	В
	ATOM	2850	õ	ARG	47	38.091 -		53.702	1.00 35.14	В
	MOTA	2851	N	LYS	48	39.054 -	-15.178	52.420	1.00 34.57	В
35	ATOM	2852	CA	LYS	48	38.456 -		53.125	1.00 32.91	В
	MOTA	2853	CB	LYS	48	36.938 -		53.092	1.00 34.16	В
	MOTA	2854	œ	LYS	48	36.361 -		51.693	1.00 36.73	B B
	MOTA	2855	CD	LYS	48 48	34.854 - 34.338 -		51.706 50.314	1.00 37.41	В
40	ATOM ATOM	2856 2857	CE NZ	LYS	48	34.704 -		49.344	1.00 36.20	В
,,	ATOM	2858	c	LYS	48	38.903 -		54.578	1.00 31.33	В
	ATOM	2859	Ō	LYS	48	38.140 -		55.440	1.00 31.50	В
	MOTA	2860	N	GLU	49	40.151 -		54.836	1.00 29.95	В
45	MOTA	2861	CA	GLU	49	40.692		56.193	1.00 27.26	В
45	MOTA	2862	CB	GLU	49	41.168		56.633 56.656	1.00 28.44	B B
	MOTA	2863	CG	GLU	49 49	40.135 - 40.760 -	-16.815	56.980	1.00 28.04	В
	MOTA MOTA	2864 2865		GLU	49	40.028		56.992	1.00 29.37	В
	ATOM	2866		GLU	49	41.986		57.220	1.00 29.95	В
50	MOTA	2867	C	GLU	49	41.924		56.344	1.00 24:62	В
	MOTA	2868	0	GLU	49	42.648 -		55.395	1.00 23.41	В
	MOTA	2869	N	VAL	50	42.123		57.565	1.00 23.85	В
	ATOM	2870	CA	VAL	50	43.276		57.915	1.00 22.58	B B
55	MOTA	2871	CB CG1	VAL VAL	50 50	42.852 - 41.863 -	-10.738	58.417 59.540	1.00 20.58	В
33	MOTA MOTA	2872 2873	CG2		. 50	44.047	-9.968	58.884	1.00 19.55	В
	ATOM	2874	c	VAL	50	43.909		59.036	1.00 23.21	В
	MOTA	2875	ō	VAL	50	43.234		59.959	1.00 22.47	В
	MOTA	2876	N	SER	51	45.197	-13.286	58.923	1.00 24.22	В
60	MOTA	2877	ÇA	SER	51	45.867	-14.078	59.950	1.00 26.05	В
	MOTA	2878	CB	SER	51	46.398		59.352	1.00 26.43	В
	MOTA	2879	OG	SER	51	46.705		60.383	1.00 26.88	B B
	ATOM	2880	c	SER	51	47.013		60.579	1.00 26.62	В
65	MOTA MOTA	2881 2882	N N	SER VAL	51 52	47.893 · 46.998 ·		59.868 61.908	1.00 28.40	В
55	ATOM	2883	CA	VAL	52 52	48.000		62.657	1.00 29.10	В
	ATOM	2884	CB	VAL	52	47.311		63.640	1.00 28.02	В
	ATOM	2885		VAL	52	48.336		64.340	1.00 27.20	В
ac	ATOM	2886		VAL	52	46.341	-10.607	62.885	1.00 27.34	В
70	ATOM	2887	C	VAL	52	48.974		63.442	1.00 30.28	. B
	ATOM	2888	0	VAL	52	48.567		64.117	1.00 30.72	8
	MOTA	2889	N	ARG	53	50.265 51.276		63.342	1.00 31.46	B B
	ATOM	2890	CA	ARG	53	31.2/0	-13.118	64.070	1.00 32.95	ь

	MOTA	2891	СВ	ARG	53	52.615	-13.750	63.336	1.00 33.14	В
	ATOM	2892	CG	ARG	53	53.636	-14.706	63.926	1.00 32.63	B
	MOTA	2893	CD	ARG	53	54.575	-15.197	62.851	1.00 33.53	В
	ATOM	2894	NE	ARG	53	55.482		62.378	1.00 34.35	В
5	ATOM	2895	CZ	ARG	53		-14.140	61.161	1.00 35.36	В
5				ARG	53		-15.089	60.272	1.00 35.11	В
	MOTA	2896							1.00 36.70	В
	MOTA	2897	NH2		53		-13.162	60.838		
	MOTA	2898	С	ARG	53		-13.182	65.458	1.00 34.27	В
	MOTA	2899	0	ARG	53		-12.088	65.632	1.00 34.80	В
1.0	MOTA	2900	N	THR	54		-13.915	66.446	1.00 35.04	В
	ATOM .	2901	·CA	THR	54	50.977	-13.458	67.815	1.00 37.72	B
	MOTA	2902	CB	THR	54	49.672	-13.823	68.540	1.00 37.47	В
	MOTA	2903	OG1	THR	54	49.521	-15.244	68.581	1.00 36.02	В
	HOTA	2904	CG2	THR	54	48.484	-13.260	67.804	1.00 37.61	В
15	ATOM	2905	C	THR	54	52.141		68.586	1.00 39.85	В
	ATOM	2906	ō	THR	54	52.517		69.633	1.00 39.10	В
	ATOM	2907	N	GLY	55		-15.121	68.043	1.00 43.17	В
	ATOM	2908	CA	GLY	55		-15.791	68.727	1.00 48.23	В
		2909		GLY	55		-15.667	68.165	1.00 51.61	· В
20	ATOM		С 0	GLY	55		-14.562	67.926	1.00 52.45	В
20	MOTA	2910		GLY	56		-16.820	67.962	1.00 53.22	В
	MOTA	2911	N					67.464	1.00 54.95	В.
	MOTA	2912	CA	GLY	56	57.219				В.
	MOTA	2913	С	GLY	56		-16.365	66.052	1.00 56.66	
25	ATOM	2914	0	GLY	56		-15.450	65.611	1.00 57.44	В
25	MOTA	2915	N	LEU	57	58.366		65.346	1.00 57.72	В
	MOTA	2916	CA	LEU	57	58.693		63.972	1.00 58.30	В
	MOTA	2917	CB	LEU	57		-16.608	63.777	1.00 58.78	В
	MOTA	2918	CG	LEU	57	61.067		64.790	1.00 59.20	В
~~	MOTA	2919		LEU	57		-18.870	64.762	1.00 59.75	В
30	MOTA	2920	CD2	LEU	57	62.542		64.472	1.00 59.20	В
	MOTA	2921	С	LEU	57	58.029		62.921	1.00 58.10	В
	MOTA	2922	0	LEU	57	57.153		63.245	1.00 58.57	В
	MOTA	2923	N	ALA	58	58.450	-17.343	61.665	1.00 57.02	В
	MOTA	2924	CA	ALA	58	57.905	-18.126	60.555	1.00 55.81	В
35	MOTA	·2925	CB	ALA	58	58.473	-17.615	59.235	1.00 55.75	В
	MOTA	2926	С	ALA	58	58.193	-19.622	60.705	1.00 54.88	В
	ATOM	2927	0	ALA	58	57.350	-20.460	60.375	1.00 54.40	В
	MOTA	2928	N	ASP	59	59.386	-19.937	61.211	1.00 53.60	В
	MOTA	2929	CA	ASP	59	59.845	-21.316	61.431	1.00 51.49	В
40	ATOM	2930	CB	ASP	59	61.254	-21.290	62.050	1.00 51.99	В
	MOTA	2931	CG	ASP	59	61.807	-22.681	62.338	1.00 52.10	В
	MOTA	2932		ASP	59		-23.464	61.385	1.00 51.56	В
	MOTA	2933		ASP	59		-22.987	63.525	1.00 52.60	В
	MOTA	2934	c	ASP	59		-22.110	62.338	1.00 49.40	В
45	MOTA	2935	ō	ASP	59		-23.315	62.197	1.00 48.84	В
	MOTA	2936	N	LYS	60		-21.404	63.256	1.00 47.59	В
	MOTA	2937	CA	LYS	60		-22.021	64.208	1.00 46.47	В
	ATOM	2938	CB	LYS	60		-22.949	65.114	1.00 45.88	В
					60		-23.470	66.345	1.00 44.88	В
50	MOTA	2939	CC	LYS			-24.217	67.209	1.00 45.79	В
50	MOTA	2940	CD	LYS	60		-24.729	68.503	1.00 47.18	В
	MOTA	2941	CE	LYS	60			69.384	1.00 48.54	В
	MOTA	2942	NZ	LYS	60		-25.298		1.00 45.74	В
	ATOM	2943	C	LYS	60		-20.862	64.977		
55	ATOM	2944	0	LYS	60		-20.017	65.532	1.00 45.66	В
55	MOTA	2945	И	SER	61		-20.802	64.999	1.00 44.14	В
	MOTA	2946	CA	SER	61		-19.718	65.697	1.00 42.32	В
	MOTA	2947	CB	SER	61		-18.419	64.892	1.00 43.45	В
	MOTA	2948	OG	SER	61	54.484	-18.594	63.545	1.00 42.02	В
	MOTA	2949	С	SER	61		-19.931	65.980	1.00 40.98	В
60 ·	MOTA	2950	0	SER	61	52.679	-20.939	65.613	1.00 40.30	В
	MOTA	2951	N	SER	62	52.686	-18.954	66.669	1.00 40.63	В
	MOTA	2952	CA	SER	62	51.265	-18.944	66.992	1.00 38.79	Ð
	MOTA	2953	CB	SER	62	51.032	-18.549	.68.445	1.00 38.80	В
	MOTA	2954	OG	SER	62		-19.441	69.325	1.00 38.30	В
65	ATOM	2955	c	SER	62		-17.862	66.115	1.00 37.30	В
	ATOM	2956	ŏ	SER	62		-16.906	65.728	1.00 37.14	В
	MOTA	2957	N	ARG	63		-18.018	65.783	1.00 36.69	В
	MOTA	2958	Cλ	ARG	63		-17.017	64.959	1.00 35.86	В
	MOTA	2959	CB	ARG	63		-17.318	63.453	1.00 35.76	В
70	ATOM	2960	CG	ARG	63		-17.378	62.918	1.00 36.93	В
, 5	MOTA	2961	CD	ARG	63		-17.660	61.418	1.00 38.47	В
	ATOM		NE	ARG	63		-16.499	60.608	1.00 40.73	В
	ATOM	2962	CZ	ARG	63		-15.428	60.393	1.00 40.83	B
	N I UPI	2963	- 2	~~	03	50.005	23.420		2.22 .0.05	-

	MOTA	2964	NH1	ARG	63	51.896 -15.353 60.928 1.00 41	
	ATOM	2965	NH2	ARG	63	50.250 -14.433 59.629 1.00 40	.58 B
	ATOM	2966	C	ARG	63	47.206 -16.982 65.296 1.00 34	.60 B
		2967		ARG	63	46.656 -17.920 65.855 1.00 33	
5	MOTA		0				
)	ATOM	2968	N	LYS	64		
	MOTA	2969	ÇA	LYS	64	45.158 -15.676 65.193 1.00 31	
	MOTA	2970	CB	LYS	64	44.913 -14.444 66.056 1.00 34	
	ATOM	2971	CG	LYS	64	45.324 -14.581 67.508 1.00 36	
	ATOM	2972	CD	LYS	64	44.298 -15.378 68.279 1.00 38	.57 B
10		2973	CE	LYS	64	44.593 -15.324 69.773 1.00 39	.71 B
10	MOTA				64	43.520 -15.964 70.596 1.00 40	
	MOTA	2974	NZ	LYS			
	ATOM	2975	С	LYS	64		
	MOTA	2976	0	LYS	64	45.114 -14.604 63.045 1.00 29	
	ATOM	2977	N	THR	65	43.537 -16.156 63.470 1.00 27	
15	MOTA	2978	CA	THR	65	42.917 -16.020 62.165 1.00 24	
	ATOM	2979	CB	THR	65	43.062 -17.321 61.338 1.00 24	.86 в
	ATOM	2980		THR	65	44.442 -17.701 61.294 1.00 24	.93 B
					65	42.555 -17.120 59.912 1.00 25	
	MOTA	2981		THR		41.449 -15.688 62.319 1.00 22	
വ	ATOM	2982	C	THR	65		
20	MOTA	2983	0	THR	65	40.752 -16.313 63.095 1.00 23	
	MOTA	2984	N	TYR	66	40.999 -14.677 61.579 1.00 21	
	MOTA	2985	CA	TYR	66	39.601 -14.232 61.612 1.00 20	
	ATOM	2986	СВ	TYR	66	39.480 -12.844 62.234 1.00 18	.74 B
	MOTA	2987	CG	TYR	66	40.144 -12.695 63.581 1.00 19	.02 B
25		2988		TYR	66	41.524 -12.584 63.695 1.00 18	
23	MOTA					42.136 -12.420 64.946 1.00 19	
	ATOM	2989		TYR	66		
	MOTA	2990		TYR	66		
	ATOM	2991	CE2	TYR	66	39.986 -12.474 66.009 1.00 19	
	ATOM	2992	CZ	TYR	66	41.357 -12.367 66.109 1.00 20	
30	ATOM	2993	OH	TYR	66	41.915 -12.234 67.382 1.00 20	.35 B
	MOTA	2994	C	TYR	66	39.027 -14.136 60.195 1.00 22	.62 B
	ATOM	2995	ō	TYR	66	39.736 -13.786 59.237 1.00 22	.83 B
		2996			67	37.747 -14.464 60.058 1.00 22	
	MOTA		N	THR			
25	MOTA	2997	CA	THR	67		
35	MOTA	2998	CB	THR	67		
	MOTA	2999	OG1	THR	67	37.169 -16.854 58.576 1.00 26	
	ATOM	3000	CG2	THR	67	35.679 -15.702 57.115 1.00 25	
	ATOM	3001	С	THR	67	36.145 -13.241 58.669 1.00 23	.25 B
	ATOM	3002	ō	THR	67	35.383 -12.979 59.598 1.00 23	.74 B
40				PHE	68	36.199 -12.521 57.556 1.00 22	
40	MOTA	3003	N			35.322 -11.379 57.354 1.00 23	
	MOTA	3004	CA	PHE	68		
	ATOM	3005	CB	PHE	68		
	ATOM	3006	CG	PHE	68	36.688 -9.788 58.758 1.00 28	
	MOTA	3007	CD1	PHE	68	37.872 -10.407 59.162 1.00 31	
45	MOTA	3008	CD2	PHE	68	36.028 -8.957 59.655 1.00 30	.45 B
	MOTA	3009		PHE	68	38.397 -10.211 60.444 1.00 33	.13 B
	ATOM	3010	CE2		68	36.539 -8.749 60.947 1.00 32	.68 B
						37.733 -9.381 61.346 1.00 34	
	MOTA	3011	CZ	PHE	68		
c 0	MOTA	3012	С	PHE	68	34.664 -11.530 56.001 1.00 23	
50	MOTA	3013	0	PHE	68	34.904 -12.505 55.318 1.00 23	
	MOTA	3014	N	ASP	69	33.836 -10.560 55.625 1.00 22	
	MOTA	3015	CA	ASP	69	33.127 -10.585 54.350 1.00 23	1.38 B
	ATOM	3016	СВ	ASP	69	31.988 -9.559 54.386 1.00 23	1.05 B
	ATOM	3017		ASP	69	30.917 -9.915 55.427 1.00 23	1.94 B
55	MOTA			ASP	69	30.875 -9.341 56.538 1.00 21	
))		3018					
	MOTA	3019		ASP	69		
	MOTA	3020	C	ASP	69	34.071 -10.363 53.173 1.00 24	
	MOTA	3021	0	ASP	69	33.880 -10.931 52.082 1.00 25	
	ATOM	3022	N	MET	70	35.089 -9.539 53.405 1.00 25	
60	ATOM	3023	CA	MET	70	36.112 -9.233 52.412 1.00 26	5.18 B
~~					70	35.686 -8.073 51.517 1.00 27	7.89 B
	MOTA	3024	CB	MET			
	MOTA	3025	CG	MET	70	*******	
	MOTA	3026	SD	MET	70		
/-	ATOM	3027	CE	MET	70	32.418 -7.227 49.126 1.00 3	
65	MOTA	3028	С	MET	70	37.378 -8.801 53.150 1.00 25	
	MOTA	3029	o	MET	70	37.301 -8.187 54.206 1.00 26	5.04 B
	MOTA	3030	N	VAL	71	38.540 -9.119 52.596 1.00 2	
	ATOM				71	39.789 -8.724 53.228 1.00 2	
		3031	CA	VAL		33	
70	MOTA	3032	CB	VAL	71		
70	MOTA	3033		VAL		39.668 -10.429 55.086 1.00 2	
	ATOM	3034	CG2	VAL	71	40.726 -11.004 52.882 1.00 2	
	ATOM	3035	С	VAL	71	40.709 -8.121 52.181 1.00 2	
	ATOM	3036	ŏ	VAL	71	40.841 -8.641 51.068 1.00 2	2.79 B
			-		_		

							2 224			-
	MOTA	3037	N	PHE	72	41.356	-7.025	52.551	1.00 22.62	В
	MOTA	3038	CA	PHE	72	42.229	-6.344	51.628	1.00 22.70	В
	MOTA	3039	CB	PHE	72	41.710	-4.936	51.321	1.00 20.63	Ð
	MOTA	3040	CG	PHE	72	40.318	-4.910	50.753	1.00 18.35	B
5	ATOM	3041		PHE	72	40.056	-5.419	49.493	1.00 15.95	В
,								51.495	1.00 17.50	В
	MOTA	3042		PHE	72	39.261	-4.409			
	MOTA	3043		PHE	72	38.771	-5.435	48.986	1.00 16.14	В
	ATOM	3044	CE2	PHE	72	37.976	-4.425	50.985	1.00 17.48	В
	ATOM	3045	CZ	PHE	72	37.732	-4.939	49.729	1.00 16.21	В
10	MOTA	3046	С	PHE	72	43.626	-6.197	52.178	1.00 22.69	В
		3047	ŏ	PHE	72	43.836	-5.523	53.181	1.00 22.50	В
	MOTA								1.00 22.82	В
	MOTA	3048	N	GLY	73	44.578	-6.837	51.508		
	MOTA	3049	CA	GLY	73	45.965	-6.741	51.920	1.00 23.34	В
	ATOM	3050	С	GLY	73	46.584	-5.398	51.571	1.00 23.29	В
15	MOTA	3051	0	GLY	73	45.982	-4.561	50.885	1.00 22.64	В
	ATOM	3052	N	ALA	74	47.809	-5.199	52.037	1.00 23.40	В
	MOTA	3053	CA	ALA	74	48.531	-3.960	51.808	1.00 25.70	В
				ALA		49.891	-4.016	52.523	1.00 25.78	В
	MOTA	3054	СВ		74				1.00 26.16	B
20	MOTA	3055	С	ALA	74	48.725	-3.639	50.328		
20	ATOM	3056	0	ALA	74	49.129	-2.556	49.978	1.00 27.50	В
	MOTA	3057	N	SER	75	48.406	-4.584	49.459	1.00 27.00	В
	MOTA	3058	CA	SER	75	48.590	-4.358	48.031	1.00 28.47	В.
	ATOH	3059	CB	SER	75	48.982	-5.679	47.335	1.00 28.85	В
	ATOM	3060	OG	SER	75	48.019	-6.709	47.507	1.00 27.19	В
25					75	47.389	-3.728	47.319	1.00 27.90	В
23	MOTA	3061	Ç	SER						
	MOTA	3062	0	SER	75	47.542	-3.123	46.243	1.00 29.21	В
	MOTA	3063	N	THR	76	46.206	-3.853	47.918	1.00 26.99	В
	MOTA	3064	CA	THR	76	44:984	-3.315	47.320	1.00 25.45	В
	MOTA	3065	CB	THR	76	43.746	-3.663	48.183	1.00 23.54	В
30	ATOM	3066		THR	76	44.015	-3.345	49.545	1.00 23.44	В
-	MOTA	3067		THR	76	43.436	-5.132	48.116	1.00 24.38	₿
					76	45.034	-1.803	47.087	1.00 25.69	В
	MOTA	3068	C	THR						В
	MOTA	3069	0	THR	76	45.543	-1.041	47.922	1.00 27.74	
0.5	MOTA	3070	N	LYS	77	44.507	-1.372	45.948	1.00 24.67	В
35	MOTA	-3071	CA	LYS	77	44.496	0.044	45.619	1.00 23.51	В
	MOTA	3072	CB	LYS	77	44.804	0.234	44.133	1.00 25.56	В
	MOTA	3073	CG	LYS	77	46.192	-0.249	43.719	1.00 28.23	В
	ATOM	3074	CD	LYS	77	46.373	-0.132	42.209	1.00 31.78	В
		3075	CE	LYS	77	47.770	-0.560	41.784	1.00 33.69	В
40	MOTA								1.00 35.35	В
40	MOTA	3076	NZ	LYS	77	47.942	-0.449	40.311		
	MOTA	3077	С	LYS	77	43.150	0.677	45.956	1.00 21.23	В
	MOTA	3078	0	LYS	77	42.175	-0.023	46.154	1.00 19.65	В
	ATOM	3079	N	GLN	78	43.105	2.008	46.021	1.00 20.16	В
	ATOM	3080	CA	GLN	78	41.853	2.714	46.335	1.00 18.91	В
45	ATOM	3081	СВ	GLN	78	42.004	4.226	46.179	1.00 18.69	В
. •	MOTA	3082	CG	GLN	78	43.063	4.851	47.064	1.00 18.42	В
								48.498	1.00 17.41	В
	ATOM	3083	CD	GLN	78	42.618	4.962			
	MOTA	3084		GLN	78	42.152	3.997	49.085	1.00 20.11	В
	MOTA	3085	NE2	GLN	78	42.756	6.143	49.066	1.00 14.62	В
50	MOTA	3086	C	GLN	78	40.743	2.294	45.377	1.00 19.40	В
	MOTA	3087	0	GLN	· 78	39.609	2.059	45.788	1.00 20.13	В
	ATOM	3088	N	ILE	79	41.074	2.208	44.092	1.00 17.68	В
	MOTA	3089	CA	ILE	79	40.089	1.815	43.094	1.00 15.86	В
								41.678	1.00 15.34	В
55	MOTA	3090	СВ	ILE	79	40.727	1,779			
55	MOTA	3091		ILE	79	41.709	0.597	41.561	1.00 16.93	В
	MOTA	3092	CG1	ILE	79	39.640	1.641	40.612	1.00 14.82	В
	ATOM	3093	CD1	ILE	79	38.766	2.868	40.410	1.00 13.32	В
	MOTA	3094	С	ILE	79	39.463	0.440	43.399	1.00 14.58	В
	MOTA	3095	ō	ILE	79	38.304	0.217	43.130	1.00 15.24	В
60 ·					80	40.231	-0.479	43.969	1.00 13.09	В
00	MOTA	3096	N	ASP						
	MOTA	3097	CA	ASP	80		-1.802	44.258	1.00 12.77	В
	MOTA	3098	СB	ASP	80	40.800	-2.818	44.435	1.00 14.43	В
	MOTA	3099	CC	ASP	80	41.645	-2.953	43.204	1.00 18.24	В
	ATOM	3100		ASP	80	41.072	-2.882	42.088	1.00 18.91	В
65	MOTA	3101		ASP	80	42.874	-3.140	43.363	1.00 21.75	В
55					80	38.787	-1.829	45.487	1.00 12.00	В
	MOTA	3102	C	ASP						В
	ATOM	3103	0	ASP	80	37.878	-2.638	45.590	1.00 10.17	
	MOTA	3104	N	VAL	81	39.063	-0.938	46.430	1.00 11.87	В
	MOTA	3105	CA	VAL	81	38.261	-0.841	47.638	1.00 10.20	В
70	MOTA	3106	CB	VAL	81	38.881	0.128	48.642	1.00 9.09	В
	MOTA	3107		VAL	81	37.857	0.529	49.689	1.00 7.52	В
	ATOM	3108		VAL	81	40.071	-0.534	49.299	1.00 11.81	В
				VAL	81	36.915	-0.292	47.224	1.00 10.85	В
	MOTA	3109	С	AVT	οŢ	50.513	0.432		2.00 10.03	-

	MOTA	3110	0	VAL	81	35.879	-0.728	47.697	1.00 11.76	В
										В.
	MOTA	3111	N	TYR	82	36.948	0.681	46.326	1.00 12.12	
	MOTA	3112	CA	TYR	82	35.735	1.304	45.845	1.00 13.85	В
_	ATOM	3113	CB	TYR	82	36.090	2.534	45.015	1.00 15.89	В
5	ATOM	3114	CG	TYR	82	34.870	3.259	44.530	1.00 18.66	В
_	MOTA	3115		TYR	82	34.364	3.029	43.256	1.00 20.38	В
	MOTA	3116	CE1	TYR	82	33.201	3.645	42.824	1.00 22.59	В
	MOTA	3117	CD2	TYR	82	34.184	4.132	45.369	1.00 19.71	В
	ATOM	3118	CE2	TYR	82	33.019	4.755	44.953	1.00 22.44	В
10	ATOM	3119	cz	TYR	82	32.531	4.508	43.675	1.00 23.44	В
10										
	MOTA	3120	OH	TYR	82	31.372	5.125	43.254	1.00 25.79	В
	MOTA	3121	С	TYR	82	34.840	0.350	45.044	1.00 14.77	В
	ATOM	3122	0	TYR	82	33.635	0.211	45.331	1.00 13.77	В
	ATON	3123	N	ARG	83	35.408	-0.299	44.035	1.00 15.58	В
15										
13	MOTA	3124	CA	ARG	83	34.632	-1.236	43.220	1.00 18.14	B
	MOTA	3125	CB	ARG	83	35.517	-1.815	42.103	1.00 20.58	В
	MOTA	3126	CG	ARG	83	35.715	-0.868	40.915	1.00 23.85	В
	ATOM	3127	CD	ARG	83	36.998	-1.162	40.161	1.00 26.52	В
									1.00 30.77	В
20	MOTA	3128	NE	ARG	83	36.971	-2.428	39.436		
20	ATOM	3129	CZ	ARG	83	36.255	-2.656	38.335	1.00 33.35	В
	MOTA	3130	NH1	ARG	83	35.485	-1.703	37.818	1.00 33.79	В
	ATOM	3131	NH2	ARG	83	36.339	-3.833	37.727	1.00 33.17	В
	ATON	3132	C	ARG	83	34.009	-2.382	44.045	1.00 18.55	В
25	MOTA	3133	0	ARG	83	32.867	-2.765	43.834	1.00 19.46	В
25	MOTA	3134	N	SER	84	34.764	-2.930	44.985	1.00 17.88	В
	ATOM	3135	CA	SER	84	34.248	-4.009	45.809	1.00 17.71	В
	ATOM	3136	CB	SER	84	35.380	-4.764	46.509	1.00 20.38	В
	ATOM	3137	OG	SER	84	36.282	-5.324	45.575	1.00 25.36	В
	ATOM	3138	C	SER	84	33.298	-3.551	46.913	1.00 16.07	В
30	MOTA	3139	0	SER	84	32.241	-4.113	47.073	1.00 15.35	В
	MOTA	3140	N	VAL	85	33.685	-2.526	47.673	1.00 15.30	В
	ATOM	3141	CA	VAL	85	32.865	-2.048	48.795	1.00 14.98	В
	MOTA	3142	CB	VAL	85	33.738	-1.521	49.963	1.00 15.00	В
	ATOM	3143	CG1	VAL	85	32.849	-1.183	51.129	1.00 15.00	В
35	ATOM	3144	CG2	VAL	85	34.775	-2.556	50.383	1:00 15.18	В.
	MOTA	3145	С	VAL	85	31.828	~0.960	48.509	1.00 14.85	В
	MOTA	3146	0	VAL	85	30.652	-1.162	48.734	1.00 13.96	В
	MOTA	3147	N	VAL	86	32.283	0.184	48.008	1.00 16.21	В
	MOTA	3148	CA	VAL	86	31.409	1.313	47.740	1.00 15.47	В
40	ATOM	3149	СВ	VAL	86	32.205	2.597	47.571	1.00 15.27	В
. •	ATOM	3150		VAL	86	31.296	3.776	47.800	1.00 15.63	В
	MOTA	3151		VAL	86	33.379	2.614	48.541	1.00 16.09	В
	MOTA	3152	С	VAL	86	30.478	1.191	46.548	1.00 15.77	В
	MOTA	3153	0	VAL	86	29.295	1.506	46.680	1.00 15.71	·B
45	ATOM	3154	N	CYS	87	30.976	0.734	45.399	1.00 15.31	В
	ATOM	3155			87		0.629	44.218	1.00 17.14	В
			CA	CYS		30.121				
	MOTA	3156	CB	CYS	87	30.787	-0.168	43.108	1.00 16.23	В
	ATOM	3157	SG	CYS	87	30.003	0.173	41.511	1.00 22.71	В
	ATOM	3158	С	CYS	87	28.753	-0.001	44.488	1.00 18.54	В
50	ATOM	3159	0	CYS	87	27.752	0.494	44.050	1.00 19.06	В
50										
	ATOM	3160	N	PRO	88	28.707	-1.117	45.207	1.00 20.44	В
	MOTA	3161	CD	PRO	88	29.827	-2.005	45.536	1.00 22.48	В
	ATOM	3162	CA	PRO	88	27.422	-1.759	45.507	1.00 21.26	В
	ATOM	3163	CB	PRO	88	27.847	-3.060	46.157	1.00 21.76	В
55	ATOM	3164	CG	PRO	88	29.168	-3.337	45.512	1.00 22.69	В
	MOTA	3165	C	PRO	88	26.542	-0.890	46.434	1.00 22.59	В
	MOTA	3166	0	PRO	88	25.333	-0.797	46.254	1.00 22.78	B
	ATOM	3167	N	ILE	89	27.151	-0.273	47.446	1.00 22.51	₿
	MOTA	3168	CA	ILE	89	26.409	0.582	48.388	1.00 22.44	В
60								49.579		В
00	ATOM	3169	СВ	ILE	89	27.298	1.003		1.00 22.87	
	ATOM	3170	CG2	ILE	89	26.592	2.040	50.408	1.00 22.27	В
	ATOM	3171	CG1	ILE	89	27.607	-0.227	50.439	1.00 24.48	В
	MOTA	3172		ILE	89	28.465	0.041	51.641	1.00 26.67	В
	ATOM	3173	C	ILE	89	25.843	1.841	47.727	1.00 22.09	
65										
UJ	MOTA	3174	0	ILE	89	24.734	2.264	48.035	1.00 21.69	В
	ATOM	3175	N	LEU	90	26.607	2.450	46.829	1.00 21.87	В
	MOTA	3176	CA	LEU	90	26.122	3.640	46.157	1.00 23.17	В
	ATOM	3177	СВ	LEU	90	27.195	4.228	45.243	1.00 20.80	В
70	MOTA	3178	CG	LEU	90	26.773	5.485	44.498	1.00 18.97	В
70	MOTA	3179	CD1		90	26.169	6.492	45.446	1.00 18.16	В
	MOTA	3180	CD2	LEU	90	27.987	6.053	43.822	1.00 20.13	В
	MOTA	3181	С	LEU	90	24.891	3.282	45.334	1.00 24.49	В
	MOTA								1.00 24.70	В
	V 1 OU	3182	0	LEU	90	23.963	4.091	45.207	1.00 44.70	ь

	MOTA	3183	N	ASP	91	24.887	2.068	44.781	1.00 25.50	В
	ATOM	3184	CA	ASP	91	23.765	1.617	43.975	1.00 26.54	В
	MOTA	3185		ASP	91	24.042	0.258	43.331	1.00 27.25	В
			CB		91		0.373	42.045	1.00 29.15	В
5	MOTA	3186	CG	ASP		24.841			1.00 28.90	В
,	MOTA	3187		ASP	91	24.725	1.424	41.365 41.701	1.00 29.60	В
	HOTA NOTA	3188		ASP	91	25.559		44.848	1.00 27.48	В
		3189	C	ASP	91	22.537	1.512		1.00 28.35	В
	MOTA	3190	0	ASP	91	21.427	1.740	44.399		
10	MOTA	3191	N	GLU	92	22.736	1.185	46.115	1.00 28.27	В
10	MOTA	3192	CA	GLU	92	21.603	1.065	47.018	1.00 28.89	В
	MOTA	3193	CB	GLU	92	22.008	0.214	48.219	1.00 30.33	В
	MOTA	3194	CG	GLU	92	20.839	-0.266	49.057	1.00 33.34	В
	MOTA	3195	CD	GLU	92	21.141		49.772	1.00 35.27	В
15	MOTA	3196		GLU	92	20.340	-2.000	50.633	1.00 36.65	В
13	MOTA	3197		GLU	92	22.181	-2.200	49.469		В
	MOTA	3198	C	GLU	92.	21.106	2.459	47.424	1.00 28.34	В
	MOTA	3199	0	GLU	92	19.897	2.685	47.581	1.00 27.53	B B
	ATOM	3200	N	VAL	93	22.037	3.395	47.585		
20	MOTA	3201	CA	VAL	93	21.663	4.757	47.938	1.00 26.25	В
20	MOTA	3202	CB	VAL	93	22.902	5.681	48.072	1.00 27.41	B B
	MOTA	3203		VAL	93	22.455	7.125	48.357	1.00 27.55	В
	MOTA	3204		VAL	93	23.807	5.170	49.178	1.00 29.02	₿.
	MOTA	3205	C	VAL	93	20.771	5.339 5.955	46.843 47.110	1.00 24.60	. B
25	HOTA	3206	0	VAL	93	19.759			1.00 22.93	В
23	MOTA	3207	N	ILE	94	21.175	5.150 5.657	45.596 44.466	1.00 23.06	В
	MOTA	3208	CA	ILE	94	20.398	5.441	43.130	1.00 22.09	В
	MOTA	3209	CB	ILE	94 94	21.193 20.367	5.867	41.905	1.00 18.23	В
	MOTA	3210		ILE	94	22.498	6.262	43.205	1.00 20.00	В
30	MOTA MOTA	3211 3212		ILE	94	23.382	6.115	42.021	1.00 18.08	В
50	ATOM	3212	CDI	ILE	94	18.984	5.036	44.384	1.00 23.71	8
	MOTA	3214	o	ILE	94	18.079	5.630	43.845	1.00 24.46	В
	ATOM	3215	N	MET	95	18.787	3.839	44.924	1.00 25.14	В
	MOTA	3216	CA	MET	95	17.451	3.234	44.893	1.00 25.03	В
35 [.]	ATOM	.3217	CB	MET	95	17.511	1.735	45.167	1.00 24.81	В
33	MOTA	3218	CG	MET	95	17.896	0.898	43.984	1.00 24.81	В
•	ATOM	3219	SD	MET	95	17.840	-0.821	44.434	1.00 28.44	В
	ATOM	3220	CE	MET	95	19.568	-1.182	44.778	1.00 27.32	В
	ATOM	3221	C	MET	95	16.585	3.864	45.977	1.00 25.84	В
40	MOTA	3222	ō	MET	95	15.407	3.606	46.068	1.00 26.55	В
	ATOM	3223	N	GLY	96	17.193	4.694	46.811	1.00 26.29	В
	ATOM	3224	CA	GLY	96	16.417	5.335	47.854	1.00 26.67	В
	MOTA	3225	c	GLY	96	16.650	4.824	49.264	1.00 28.04	В
	MOTA	3226	ō	GLY	96	15.864	5.121	50.170	1.00 29.08	В
45	ATOM	3227	N	TYR	97	17.733	4.075	49.454	1.00 28.81	В
	ATOM	3228	CA	TYR	97	18.081	3.524	50.760	1.00 29.52	В
	ATOM	3229	CB	TYR	97	18.680	2.117	50.591	1.00 31.73	В
	ATOM	3230	CG	TYR	97	17.674	1.041	50.230	1.00 34.37	В
	ATOM	3231		TYR	97	17.016	0.310	51.223	1.00 35.37	В
50	ATOM	3232		TYR	97	16.087	-0.663	50.904	1.00 36.70	В
	ATOM	3233		TYR	97	17.370	0.769	48.901	1.00 35.61	В
	MOTA	3234		TYR	97	16.439	-0.198	48.569	1.00 37.43	В
	ATOM	3235	CZ	TYR	97	15.800	-0.909	49.575	1.00 38.91	В
	ATOM	3236	ОН	TYR	97	14.858	-1.862	49.257	1.00 40.43	В
55	MOTA	3237	С	TYR	97	19.090	4.391	51.528	1.00 28.25	В
	ATOM	3238	0	TYR	97	19.819	5.172	50.943	1.00 29.03	В
	ATON	3239	N	ASN	98	19.107	4.266	52.850	1.00 26.29	В
	ATOM	3240	CA	ASN	98	20.087	4.993	53.646	1.00 24.16	В
	MOTA	3241	CB	ASN	98	19.520	5.396	54.994	1.00 23.70	В
60 ·	ATOM	3242	CG	ASN	98	18.552	6.526	54.883	1.00 21.81	В
	ATOM	3243	OD1	ASN	98	18.764	7.475	54.138	1.00 20.22	В
	ATOM	3244	ND2	ASN	98	17.483	6.442	55.642	1.00 22.90	В
	ATOM	3245	С	ASN	98	21.262	4.051	53.883	1.00 22.53	В
	ATOM	3246	ō	ASN	98	21.076	2.860	54.149	1.00 23.91	В
65	MOTA	3247	N	CYS	99	22.475	4.573	53.770	1.00 20.08	В
	ATOM	3248	CA	CYS	99	23.652	3.741	53.976	1.00 16.35	В
	ATOM	3249	CB	CYS	99	24.239	3.318	52.641	1.00 16.30	В
	ATOM	3250	SG	CYS	99	23.128	2.271	51.748	1.00 16.76	В
	ATOM	3251	C	CYS	99	24.717	4.437	54.786	1.00 13.97	В
70	MOTA	3252	ō	CYS	99	24.764	5.664	54.867	1.00 13.48	В
	ATOM	3253	N	THR	100	25.584	3.631	55.374	1.00 12.82	В
	MOTA	3254	CA	THR	100	26.646	4.149	56.209	1.00 10.88	В
	ATOM	3255	CB	THR	100 -	26.177	4.209	57.660	1.00 9.58	В

	MOTA	3256	0G1	THR	100	25.155	5.204	57.768	1.00 6.29	В
	ATOM	3257		THR	100	27.327	4.524	58.590	1.00 10.26	В
					100	27.874	3.264	56.104	1.00 10.53	В
	ATOM	3258	C	THR						В
5	MOTA	3259	0	THR	100	27.764	2.056	56.040	1.00 10.24	
5	MOTA	3260	N	ILE	101	29.044	3.890	56.059	1.00 10.89	В
	MOTA	3261	CA	ILE	101	30.303	3.156	55.993	1.00 12.11	В
	MOTA	3262	CB	ILE	101	31.004	3.297	54.642	1.00 13.63	В
	ATOM	3263	CG2	ILE	101	32.258	2.424	54.623	1.00 13.65	В
	ATOM	3264	CG1		101	30.057	2.935	53.504	1.00 15.35	В
10	MOTA	3265	CDI	ILE	101	30.607	3.332	52.135	1.00 15.19	В
10										В
	MOTA	3266	C	ILE	101	31.226	3.776	57.027	1.00 11.10	
	MOTA	3267	0	ILE	101	31.518	4.944	56.962	1.00 13.95	В
	MOTA	3268	N	PHE	102	31.690	2.961	57.960	1.00 8.97	В
	MOTA	3269	CA	PHE	102	32.569	3.412	59.024	1.00 5.36	В
15	MOTA	3270	CB	PHE	102	32.254	2.693	60.337	1.00 5.27	В
	MOTA	3271	CG	PHE	102	30.964	3.097	60.979	1.00 3.08	В
	MOTA		. CD1		102	30.912	4.233	61.785	1.00 3.17	В
	MOTA	3273		PHE	102	29.821	2.315	60.839	1.00 1.92	В
	MOTA							62.458	1.00 2.33	В
20		3274	CE1	PHE	102	29.737	4.591			
20	MOTA	3275		PHE	102	28.648	2.667	61.505	1.00 1.69	В
	MOTA	3276	CZ	PHE	102	28.608	3.812	62.323	1.00 1.17	В
	MOTA	3277	c	PHE	102	33.974	2.937	58.708	1.00 4.97	В
	MOTA	3278	0	PHE	102	34.160	1.984	57.99 7	1.00 6.23	В
	MOTA	3279	N	ALA	103	34.956	3.641	59.244	1.00 5.31	В
25	MOTA	3280	CA	ALA	103	36.345	3.256	59.091	1.00 3.70	В
	ATOM	3281	CB	ALA	103	37.115	4.337	58.408	1.00 2.97	В
	ATOM	3282	C	ALA	103	36.781	3.126	60.546	1.00 3.79	В
										В
	MOTA	3283	0	ALA	103	36.811	4.105	61.266	1.00 4.80	
20	MOTA	3284	N	TYR	104	37.086	1.908	60.981	1.00 3.80	В
30	ATOM	3285	CA	TYR	104	37.503	1.670	62.366	1.00 3.56	В
	MOTA	3286	CB	TYR	104	36.507	0.751	63.061	1.00 2.47	В
	MOTA	3287	CG	TYR	104	36.842	0.498	64.507	1.00 1.59	В
	MOTA	3288		TYR	104	37.780	-0.465	64.875	1.00 1.99	В
	MOTA	3289		TYR	104	38.079	-0.706	66.227	1.00 1.00	В
35	ATOM	3290		TYR	104	36.211	1.215	65.510	1.00 3.23	В
23		3291				36.492		66.863	1.00 1.00	В
	MOTA		CE2	TYR	104		0.988			
	MOTA	3292	CZ	TYR	104	37.419	0.031	67.217	1.00 1.00	В
	MOTA	3293	OH	TYR	104	37.667	-0.164	68.555	1.00 1.00	В
40	MOTA	3294	С	TYR	104	38.893	1.046	62.517	1.00 3.38	В
40	MOTA	3295	0	TYR	104	39.225	0.087	61.843	1.00 3.35	В
	ATOM	3296	N	GLY	105	39.680	1.586	63.440	1.00 4.31	В
	MOTA	3297	CA	GLY	105	41.024	1.088	63.646	1.00 5.04	В
	MOTA	3298	С	GLY	105	41.931	2.086	64.335	1.00 5.61	В
	ATOM	3299	ō	GLY	105	41.560	3.226	64.565	1.00 5.55	В
45	ATOM	3300	N		106	43.132	1.627	64.657	1.00 7.21	В
45				GLN						В
	MOTA	3301	CA	GLN	106	44.154	2.414	65.338	1.00 9.77	
	MOTA	3302	CB	GLW	106	45.303	1.473	65.701	1.00 11.84	В
	MOTA	3303	CG	GLN	106	46.625	2.127	65.977	1.00 18.02	В
	MOTA	3304	CD	GLN	106	47.651	1.110	66.407	1.00 20.93	В
50	MOTA	3305	OE1	GLN	106	47.887	0.126	65.707	1.00 20.58	B
	MOTA	3306	NE2	GLN	106	48.265	1.333	67.569	1.00 24.16	В
	MOTA	3307	С	GLN	106	44.684	3.603	64.525	1.00 9.05	В
	MOTA	3308	0	GLN	106	44.759	3.535	63.318	1.00 8.64	В
	MOTA	3309	N	THR	107	45.040	4.693	65.206	1.00 9.25	В
55						45.589		64.537	1.00 9.91	В
23	MOTA	3310	CA	THR	107		5.863			
	MOTA	3311	CB		107	46.090	6.935	65.545	1.00 11.30	В
	MOTA	3312	OG1	THR	107	44.998	7.433	66.328	1.00 12.57	₿
	ATOM	3313	CG2	THR	107	46.715	8.089	64.807	1.00 11.37	В
	ATOM	3314	С	THR	107	46.784	5.384	63.720	1.00 9.43	В
60	MOTA	3315	0	THR	107	47.631	4.615	64.226	1.00 6.62	В
•••	ATOM	3316	N	GLY	108	46.836	5.797	62.455	1.00 7.40	В
	MOTA	3317	CA	GLY	108	47.956	5.419	61.613	1.00 7.87	В
	MOTA	3318	С	GLY	108	47.801	4.136	60.815	1.00 7.55	В
10	MOTA	3319	0	GLY	108	48.771	3.609	60.263	1.00 10.21	В
65	MOTA	3320	N	THR	109	46.581	3.624	60.748	1.00 5.82	В
	MOTA	3321	CA	THR	109	46.349	2.400	59.992	1.00 4.83	В
	MOTA	3322	CB	THR	109	45.588	1.329	60.827	1.00 3.30	В
	ATOM	3323		THR	109	44.316	1.824	61.248	1.00 2.94	В
	MOTA	3324		THR	109		0.954	62.027		В
70						46.388			1.00 4.86	
10	MOTA	3325	C	THR	109	45.611	2.616	58.675	1.00 5.10	В
	MOTA	3326	0	THR	109	45.305	1.648	57.954	1.00 5.03	В
	MOTA	3327	N	GLY	110	45.298	3.871	58.364	1.00 3.29	В
	MOTA	3328	CA	GLY	110	44.613	4.141	57.122	1.00 1.90	В

	MOTA	3329	С	GLY	110	43.131	4.484	57.097	1.00 2.61	В
										В
	MOTA	3330	٥	GLY	110	42.521	4.385	56.025	1.00 1.00	
	MOTA	3331	N	LYS	111	42.539	4.885	58.227	1.00 4.13	В
		3332	CA		111	41.117	5.282	58.231	1.00 2.65	В
-	MOTA			LYS						
5	ATOM	3333	CB	LYS	111	40.636	5.636	59.651	1.00 2.73	В
	MOTA	3334	CG	LYS	111	40.588	4.463	60.630	1.00 4.22	В
	MOTA .	3335	CD	LYS	111	39.990	4.860	61.974	1.00 1.25	В
	MOTA	3336	CE	LYS	111	40.770	5.978	62.652	1.00 1.64	В
										В
10	MOTA	3337	NZ	LYS	111	42.112	5.563	63.122		
10	MOTA	3338	C	LYS	111	40.876	6.516	57.319	1.00 3.52	В
	ATOM	3339	٠0	LYS	111	39.940	6.553	56.504	1.00 3.17	В
	MOTA	3340	N	THR	112	41.738	7.515	57.421	1.00 2.71	В
	ATOM	3341	CA	THR	112	41.536	8.697	56.607	1.00 4.38	В
	MOTA	3342	CB	THR	112	42.245	9.927	57.209	1.00 3.24	В
. 15	MOTA	3343	001	THR	112	41.689	10.219	58.500	1.00 2.46	В
									1.00 5.02	B
	MOTA	3344		THR	112	42.049	11.122	56.306		
	MOTA	3345	С	THR	112	42.010	8.459	55.175	1.00 6.62	В
	MOTA	3346	0	THR	112	41.499	9.074	54.223	1.00 5.92	В
	MOTA	3347	N	PHE	113	42.974	7.556	55.013	1.00 7.30	В
20	MOTA	3348	·CA	PHE	113	43.484	7.275	53.680	1.00 9.51	В
									1.00 11.02	В
	MOTA	3349	CB	PHE	113	44.690	6.342	53.705		
	MOTA	3350	cc	PHE	113	45.299	6.119	52.344	1.00 13.48	В
	MOTA	3351	CDI	PHE	113	46.106	7.088	51.763	1.00 13.42	В
	MOTA	3352	CD2	PHE	113	45.021	4.974	51.624	1.00 13.65	В
25	MOTA	3353	CE1	PHE	113	46.626	6.927	50.496	1.00 13.19	В
										В
	ATOM	3354		PHE	113	45.542	4.806	50.345	1.00 14.93	
	MOTA	3355	CZ	PHE	113	46.346	5.792	49.784	1.00 13.30	В
	ATOM	3356	С	PHE	113	42:393	6.604	52.866	1.00 10.02	В
	MOTA	3357	0	PHE	113	42.195	6.916	51.689	1.00 9.19	В
30	MOTA	3358	N	THR	114	41.686	5.686	53.519	1.00 9.92	В
-										
	MOTA	3359	CA	THR	114	40.601	4.946	52.905	1.00 8.86	В
	ATOM	3360	CB	THR	114	40.157	3.792	53.812	1.00 9.97	В
	MOTA			THR	114	41.256	2.900	54.000	1.00 10.04	В
		3361								
	ATOM	3362	CG2	THR	114	39.026	3.006	53.174	1.00 10.07	В
35	ATOM	.3363	С	THR	114	39.397	5.824	52.608	1.00 8.06	В
	MOTA	3364	0	THR	114	38.935	5.875	51.496	1.00 8.14	В
	MOTA	3365	N	MET	115	38.908	6.538	53.612	1.00 6.57	В
	MOTA		CA	MET	115	37.730	7.365	53.422	1.00 6.18	В
		3366								
	MOTA	3367	CB.	MET	115	37.149	7.844	54.760	1.00 8.16	В
40	ATOM	3368	CG	MET	115	36.761	6.723	55.717	1.00 12.31	В
	MOTA	3369	SD	MET	115	35.709	5.494	54.920	1.00 17.76	В
	MOTA	3370	CE	MET	115	34.142	6.334	54.973	1.00 16.39	В
	MOTA	3371	C	MET	115	37.903	8.594	52.570	1.00 6.31	В
	MOTA	3372	0	MET	115	36.998	8.943	51.837	1.00 10.20	В
45	MOTA	3373	N	GLU	116	39.061	9.244	52.660	1.00 6.06	В
										В
	MOTA	3374	CA	GLU	116	39.295	10.476	51.909	1.00 2.45	
	MOTA	3375	CB	GLU	116	39.743	11.607	52.838	1.00 2.23	В
	MOTA	3376	CG			38.737	11.962	53.924	1.00 1.00	B
	MOTA	3377	CD	GLU	116	39.091	13.216	54.722	1.00 1.00	В
50	MOTA	3378	OE1	GLU	116	40.124	13.850	54.464	1.00 1.56	B
-										В
	MOTA	3379	UEZ	GLU	116	38.323	13.586	55.626	1.00 1.00	
	MOTA	3380	С	GLU	116	40.342	10.311	50.843	1.00 2.04	В
	MOTA	3381	0	GLU	116	40.070	10.587	49.695	1.00 1.54	В
	MOTA	3382	N	GLY	117	41.539	9.869	51.235	1.00 2.71	В
55	MOTA	3383	CA	GLY	117	42.603	9.663	50.263	1.00 3.19	B
	MOTA						10.842	50.294		В
	ATOM	3384	С	GLY	117	43.531			1.00 1.91	
	ATOM	3385	٥	GLY	117	43.293	11.739	51.033	1.00 2.28	В
	MOTA	3386	N	GLU	118	44.568	10.822	49.466	1.00 3.14	В
	MOTA	3387	CA	GLU	118	45.562	11.897	49.412	1.00 3.61	В
60	MOTA	3388	CB	GLU	118	46.879	11.427	50.051	1.00 3.14	В
	ATOM	3389	CG	GLU	118	46.652	10.690	51.389	1.00 7.09	В
	MOTA	3390	CD	GLU	118	47.933	10.200	52.062	1.00 9.57	В
							9.748	51.317	1.00 11.82	В
	ATOM	3391		GLU	118	48.831				
	ATOM	3392	OE2	GLU	118	48.030	10.259	53.317	1.00 6.51	В
65	ATOM	3393	C	GLU	118	45.813	12.253	47.959	1.00 4.59	В
0.5										
	MOTA	3394	0	GLU	118	45.209	11.670	47.063	1.00 4.23	В
	MOTA	3395	N	ARG	119	46.681	13.221	47.713	1.00 7.04	В
	MOTA	3396	CA	ARG	119	46.976	13.564	46.329	1.00 10.62	В
	MOTA	3397	CB	ARG	119	47.171	15.067	46.131	1.00 10.38	В
70									1.00 13.02	В
,,,	MOTA	3398	CG	ARG	119	45.961	15.941	46.462		
	MOTA	3399	CD	ARG	119	44.705	15.414	45.837	1.00 13.25	В
	MOTA	3400	NE	ARG	119	44.838	15.093	44.420	1.00 13.98	В
	MOTA	3401	CZ	ARG	119	44.759	15.955	43.411	1.00 11.43	В

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	MOTA	3402		ARG	119	44.543	17.247	43.614	1.00 9.13	В
	ATOM	3403	NH2		119	44.890	15.498	42.175	1.00 10.86	В
	MOTA	3404	С	ARG	119	48.274	12.907	45.912	1.00 12.67	В
~	MOTA	3405	0	ARG	119	49.210	12.823	46.712	1.00 12.43	В
5	MOTA	3406	N	SER	120	48.328	12.416	44.675	1.00 15.44	В
	MOTA	3407	CA	SER	120	49.563	11.812	44.182	1.00 17.48	В
	MOTA	3408	CB	SER	120	49.392	11.272	42.755	1.00 18.24	В
	MOTA	3409	OG	SER	120	48.605	10.090	42.735	1.00 19.78	В
• •	MOTA	3410	С	SER	120	50.519	12.978	44.185	1.00 18.56	В
10	MOTA	3411	0	SER	120	50.161	14.050	43.772	1.00 20.75	В
	MOTA	3412	N	PRO	121	51.748	12.782	44.660	1.00 20.06	В
	MOTA	3413	CD	PRO	121	52.403	11.508	45.013	1.00 20.52	В
	MOTA	3414	CA	PRO	121	52.700		44.686	1.00 20.89	В
1.5	MOTA	3415	СВ	PRO	121	53.912	13.275	45.385	1.00 21.27	В
15	MOTA	3416	CG	PRO	121	53.881	11.834	44.872	1.00 21.35	В
	MOTA	3417	С	PRO	121	53.028	14.538	43.332	1.00 21.75	В
	MOTA	3418	0	PRO	121	52.835	13.918	42.270	1.00 21.17	В
•	MOTA	3419	И	ASN	122	53.514	15.785	43.393	1.00 21.50	В
20	MOTA	3420	CA	ASN	122	53.957	16.561	42.227	1.00 22.52	В
20	MOTA	3421	CB	ASN	122	55.199	15.865	41.632	1.00 24.29	В
	MOTA	3422	CG	ASN	122	56.137	16.828	40.956	1.00 26.30	В
	MOTA	3423		ASN	122	56.538	17.815	41.553	1.00 28.88	В
	MOTA	3424		ASN	122	56.488	16.552	39.705	1.00 26.63	В
25	MOTA	3425	C	ASN	122	52.917	16.852	41.126	1.00 22.37	. B
23	MOTA	3426	0	ASN	122	53.271	16.962	39.930	1.00 20.20 1.00 22.38	В
	MOTA	3427	N	GLU	123	51.651	16.999 17.294	41.518 40.561	1.00 22.38	B
	MOTA	3428 3429	CA	GLU	123	50.573 50.664	18.735	40.072	1.00 21.58	В
	MOTA MOTA	3430	CB	GLU	123 123	50.338	19.754	41.110	1.00 21.60	В
30				GLU	123	50.218	21.112	40.506	1.00 23.71	В
50	MOTA MOTA	3431 3432	CD	GLU	123	51.124	21.512	39.736	1.00 24.05	В
		. 3433		GLU	123	49.220	21.789	40.808	1.00 24.70	B
	MOTA	3434	C	GLU	123	50.573	16.401	39.319	1.00 23.43	В
-	ATOM	3435	ŏ	GLU	123	50.357	16.856	38.189	1.00 22.15	В
35	ATOM	3436	N	GLU	124	50.809	15.116	39.538	1.00 25.66	В
	MOTA	3437	CA	GLU	124	50.840	14.186	38.435	1.00 27.17	В
	ATOM	3438	CB	GLU	124	51.320	12.816	38.905	1.00 28.99	В
	ATOM	3439	CG	GLU	124	51.698	11.884	37.763	1.00 33.91	В
	MOTA	3440	CD	GLU	124	52.179	10.531	38.247	1.00 36.81	В
40	MOTA	3441	OE1	GLU	124	52.681	10.475	39.395	1.00 37.60	В
	MOTA	3442	OE2	GLU	124	52.061	9.543	37.476	1.00 36.71	В
	ATOM	3443	С	GLU	124	49.466	14.045	37.791	1.00 26.54	В
	MOTA	3444	0	GLU	124	49.351	13.966	36.571	1.00 28.04	В
	MOTA	3445	N	TYR	125	48.425	14.023	38.616	1.00 24.51	B
45	MOTA	3446	CA	TYR	125	47.065	13.864	38.117	1.00 22.37	В
	MOTA	3447	CB	TYR	. 125	46.424	12.570	38.618	1.00 24.02	В
	MOTA	3448	CG	TYR	125	47.232	11.305	38.445	1.00 24.34	В
	MOTA	3449		TYR	125	48.215	10.951	39.372	1.00 24.16	В
50	MOTA	3450		TYR	125	48.938	9.770	39.238	1.00 24.97	В
30	MOTA	3451		TYR	125	46.994	10.440	37.368	1.00 23.29 1.00 23.28	B B
	ATOM	3452		TYR	125	47.715	9.257 8.927	37.224 38.165	1.00 25.16	В
	MOTA	3453	CZ	TYR	125	48.685	7.750	38.059	1.00 24.88	В
	ATOM	3454	ОН	TYR	125	49.395	14.936	38.586	1.00 22.58	В
55	MOTA MOTA	3455 3456	C	TYR TYR	125 125	46.366	15.703	39.516	1.00 24.23	В
55	ATOM	3457	0 N	THR	126	44.941	14.984	37.920	1.00 21.47	В
	ATOM	3458	CA	THR	126	43.889	15.919	38.280	1.00 20.00	В
	ATOM	3459	CB	THR	126	42.913	16.147	37.140	1.00 20.72	В
	ATOM	3460		THR	126	42.379	14.888	36.723	1.00 21.10	В
60	ATOM	3461		THR	126	43.598	16.837	35.984	1.00 20.85	В
	ATOM	3462	C	THR	126	43.158	15.142	39.353	1.00 17.64	В
	ATOM	3463	ŏ	THR	126	43.223	13.940	39.359	1.00 16.55	В
	ATOM	3464	N	TRP	127	42.441	15.820	40.241	1.00 16.83	В
	ATOM	3465	CA	TRP	127	41.749	15.118	41.332	1.00 15.87	В
65	ATOM	3466	СВ	TRP	127	40.927	16.080	42.213	1.00 14.78	В
	ATOM	3467	CG	TRP	127	39.645	16.561	41.596	1.00 12.27	В
	MOTA	3468		TRP	127	38.379	15.935	41.708	1.00 9.16	В
	MOTA	3469		TRP	127	37.467	16.702	40.951	1.00 9.12	В
	MOTA	3470		TRP	127	37.925	14.802	42.375	1.00 7.09	В
70	ATOM	3471		TRP	127	39.462	17.662	40.795	1.00 11.95	В
	MOTA	3472	NE1	TRP	127	38.150	17.749	40.405	1.00 11.09	В
	MOTA	3473		TRP	127	36.142	16.366	40.845	1.00 B.67	В
	MOTA	3474	CZ3	TRP	127	36.606	14.472	42.271	1.00 7.96	В

		3435	0113		127	25 724		41 511	1 00 0 13	В
	MOTA	3475		TRP	127	35.724	15.251	41.511	1.00 9.12	В
	MOTA	3476	C	TRP TRP	127 127	40.824 40.807	13.969 12.907	40.917 41.536	1.00 15.77 1.00 16.78	В
	MOTA MOTA	3477 3478	O N	GLU	128	40.807	14.145	39.855	1.00 16.83	В
5	MOTA	3479	CA	GLU	128	39.168	13.073	39.465	1.00 16.42	В
3	ATOM	3480	СВ	GLU	128	38.092	13.631	38.537	1.00 15.75	В
	ATOM	3481	CG	GLU	128	38.578	14.230	37.234	1.00 14.47	B
	ATOM	3482	CD	GLU	128	37.432	14.890	36.478	1.00 17.33	В
	ATOM	3483		GLU	128	36.986	15.975	36.897	1.00 18.91	В
10	ATOM	3484		GLU	128	36.954	14.324	35.477	1.00 17.86	В
	ATOM	3485	·C	GLU	128	39.828	11.828	38.847	1.00 17.44	В
	MOTA	3486	0	GLU	128	39.142	10.851	38.564	1.00 17.96	В
	MOTA	3487	N	GLU	129	41.147	11.846	38.653	1.00 18.02	В
	MOTA	3488	CA	GLU	129	41.836	10.692	38.078	1.00 19.12	В
15	MOTA	3489	CB	GLU	129	42.509	11.020	36.740	1.00 20.74	В
	MOTA	3490	CG	GLU	129	41.574	11.402	35.595	1.00 26.16	В
	MOTA	3491	CD	GLU	129	42.324	11.739	34.299	1.00 30.95	B B
	MOTA	3492		GLU	129	41.711	12.357	33.393	1.00 32.49	В
20	MOTA MOTA	3493 3494	C	GLU	129 129	43.521 42.945	11.385. 10.219	38.990	1.00 18.40	В
20	ATOM	3495	ò	GLU	129	43.677	9.331	38.637	1.00 18.01	В
	ATOM	3496	N	ASP	130	43.051	10.816	40.173	1.00 17.65	В.
	MOTA	3497	CA	ASP	130	44.115	10.465	41.113	1.00 17.80	В
	ATOM	3498	CB	ASP	130	44.200	11.536	42.211	1.00 17.64	·B
25	ATOM	3499	CG	ASP	130	45.540	11.556	42.908	1.00 19.83	В
	MOTA	3500	OD1	ASP	130	46.026	10.466	43.291	1.00 20.74	В
	MOTA	3501	OD2	ASP	130	46.097	12.661	43.070	1.00 20.64	В
	MOTA	3502	С	ASP	130	43:843	9.091	41.704	1.00 17.66	В
20	MOTA	3503	0	ASP	130	42.792	8.867	42.302	1.00 18.25	В
30	MOTA	3504	N	PRO	131	44.778	8.141	41.521	1.00 17.22	В
	MOTA	3505	CD	PRO	131	46.046	8.282 6.778	40.780 42.052	1.00 17.06 1.00 16.05	B B
	MOTA MOTA	3506 3507	CA CB	PRO PRO	131 131	44.617 45.716	5.994	41.316	1.00 14.70	В
	MOTA	3508	CG	PRO	131	46.802	7.019	41.154	1.00 17.48	В
35	MOTA	.3509	c	PRO	131	44.668	6.713	43.589	1.00 15.30	В
	MOTA	3510	ō	PRO	131	44.318	5.697	44.187	1.00 14.37	В
	MOTA	3511	N	LEU	132	45.114	7.797	44.226	1.00 15.18	В
	MOTA	3512	CA	LEU	132	45.169	7.841	45.683	1.00 13.57	. В
٠.	MOTA	3513	CB	LEU	132	46.380	B.644	46.165	1.00 12.21	В
40	MOTA	3514	CG	LEU	132	47.741	8.012	45.842	1.00 12.83	В
	MOTA	3515		LEU	132	48.850 47.773	8.803 6.553	46.511 46.317	1.00 7.88 1.00 13.99	B B
	MOTA MOTA	3516 3517	CD2	LEU LEU	132 132	43.882	8.393	46.295	1.00 14.28	В
	MOTA	3518	ō	LEU	132	43.737	8.410	47.526	1.00 13.98	В
45	ATOM	3519	N	ALA	133	42.947	8.832	45.443	1.00 13.83	В
	MOTA	3520	CA	ALA	133	41.651	9.342	45.909	1.00 12.82	В
	MOTA	3521	CB	ALA	133	40.796	9.805	44.733	1.00 12.54	В
	ATOM	3522	С	ALA	133	40.875	8.291	46.717	1.00 13.00	В
50	MOTA	3523	0	ALA	133	40.840	7.092	46.371	1.00 14.00	В
50	MOTA	3524	N	GLY	134	40.226	8.760	47.780	1.00 13.17	В
	MOTA	3525	CA	GLY	134	39.470	7.884	48.653	1.00 10.45	B B
	MOTA	3526	C	GLY	134 134	37.996 37.546	7.819 8.422	48.324 47.385	1.00 9.48 1.00 8.50	В
	MOTA MOTA	3527 3528	N	ILE	135	37.254	7.094	49.158	1.00 10.67	В
55	MOTA	3529	CA	ILE	135	35.820	6.874	48.981	1.00 9.46	В
	ATOM	3530	СВ	ILE	135	35.237	6.087	50.180	1.00 9.70	В
	MOTA	3531		ILE	135	33.709	5.990	50.079	1.00 10.21	В
	ATOM	3532		ILE	135	35.837	4.686	50.214	1.00 8.19	В
	MOTA	3533	CD1	ILE	135	35.426	3.864	51.452	1.00 8.61	В
60	MOTA	3534	С	ILE	135	34.968	8.115	48.739	1.00 9.92	В
	MOTA	3535	0	ILE	135	34.135		47.812	1.00 7.51	В
	MOTA	3536	N	ILE	136	35.157	9.136	49.560	1.00 9.63	В
	MOTA	3537	CA	ILE	136	34.379	10.340	49.371	1.00 8.14	В
65	MOTA	3538	CB	ILE	136	34.671	11.371	50.500	1.00 6.28	B B
55	MOTA	3539 3540		ILE	136 136	33.997 34.125	10.825	50.166 51.831	1.00 6.74 1.00 5.22	В
	MOTA MOTA	3540		ILE	136	34.553	11.574	53.070	1.00 1.00	В
	MOTA	3542	C	ILE	136	34.538	10.992	47.978	1.00 9.33	В
	MOTA	3543	ŏ	ILE	136	33.569	11.242	47.274	1.00 10.23	В
70	MOTA	3544	N	PRO	137	35.767	11.252	47.552	1.00 7.86	В
	MOTA	3545	CD	PRO	137	37.096	11.215	48.163	1.00 7.00	B
	MOTA	3546	CA	PRO	137	35.816	11.874	46.234	1.00 7.00	В
	MOTA	3547	CB	PRO	137	37.243	12.398	46.174	1.00 5.68	В

	MOTA	3548	CG	PRO	137	37.968	11.448	46.976	1.00 7.36	В
	MOTA	3549	c	PRO	137	35.370	10.967	45.098	1.00 7.27	В
	ATOM	3550	ŏ	PRO	137	34.857	11.434	44.120	1.00 9.92	В
	ATOM	3551	N	ARG	138	35.547	9.661	45.233	1.00 7.38	В
5	MOTA	3552	CA	ARG	138	35.132	8.765	44.157	1.00 4.69	В
-	MOTA	3553	CB	ARG	138	35.761	7.375	44.314	1.00 5.18	В
	ATOM	3554	CG	ARG	138	37.257	7.373	44.145	1.00 4.97	В
	MOTA	3555	CD	ARG	138	37.858	6.057	44.522	1.00 8.61	В
	ATOM	3556	NE	ARG	138	39.307	6.094	44.387	1.00 9.73	В
10	ATOM	3557	CZ	ARG	138	39.954	5.973	43.235	1.00 12.02	В
	MOTA	3558	NH1	ARG	138	39.279	5.799	42.102	1.00 12.04	В
	MOTA	3559	NH2	ARG	138	41.280	6.028	43.216	1.00 13.69	В
	MOTA	3560	С	ARG	138	33.623	8.667	44.131	1.00 4.18	В
	MOTA	3561	0	ARG	138	33.017	8.611	43.094	1.00 7.46	В
15	MOTA	3562	N	THR	139	33.013	8.666	45.295	1.00 3.72	В
	MOTA	3563	CA	THR	139	31.578	8.581	45.339	1.00 3.48	B
	MOTA	3564	CB	THR	139	31.103	8.436	46.792	1.00 2.17	В
	MOTA	3565		THR	139	31.647	7.220	47.321	1.00 4.08	В
20	MOTA	3566		THR	139	29:586	8.366	46.872	1.00 1.00	B B
20	MOTA	3567	C	THR	139	30.956	9.798	44.677	1.00 4.20 1.00 5.38	В
	MOTA	3568	0	THR	139	30.178	9.666	43.727 45.148	1.00 5.38 1.00 4.85	8
	ATOM	3569	N	LEU	140	31.313	10.983	44.582	1.00 5.86	В
	ATOM	3570	CA	LEU	140	30.740 31.374	12.187 13.423	45.207	1.00 4.02	8
25	MOTA	3571	CB	LEU	140 140	30.995	13.484	46.692	1.00 4.42	В
23	ATOM	3572 3573	CG CD1	LEU	140	31.695	14.631	47.363	1.00 6.86	. в
	MOTA MOTA	3574		LEU	140	29.511	13.617	46.827	1.00 2.19	В
	MOTA	3575	CD2	LEU	140	30.902	12.211	43.091	1.00 8.32	В
	MOTA	3576	ō	LEU	140	29.958	12.523	42.378	1.00 10.70	В
30	ATOM	3577	N	HIS	141	32.085	11.853	42.611	1.00 9.41	В
	ATOM	3578	CA	HIS	141	32.315	11.876	41.180	1.00 11.42	В
	ATOM	3579		HIS	141	33.753	11.465	40.836	1.00 12.95	В
	ATOM	3580	CG	HIS	141 -	34.064	11.523	39.364	1.00 15.31	В
	MOTA	3581	CD2	HIS	141	34.074	10.555	38.413	1.00 14.59	В
35	MOTA	3582	ND1	HIS	141	34.404	12.693	38.713	1.00 17.05	В
	MOTA	3583	CE1	HIS	141	34.612	12.445	37.432	1.00 15.66	В
	ATOM	3584	NE2	HIS	141	34.418	11.154	37.225	1.00 15.55	В
	ATOM	3585	С	HIS	141	31.362	10.910	40.495	1.00 11.46	В
40	ATOM	3586	0	HIS	141	30.727	11.239	39.499	1.00 12.67	B.
40	MOTA	3587	N	GLN	142	31.251	9.714	41.054	1.00 12.56	B B
	ATOM	3588	CA	GLN	142	30.405	8.694	40.464	1.00 12.86	В
	MOTA	3589	CB	GLN	142	30.707	7.336	41.103 40.590	1.00 14.25	В
	MOTA	3590	CG	GLN	142	32.000 32.012	6.739 6.628	39.068	1.00 21.75	В
45	ATOM	3591 3592	CD	GLN GLN	142 142	31.349	5.751	38.489	1.00 23.11	В
73	MOTA MOTA	3593		GLN	142	32.743	7.535	38.408	1.00 20.86	В
	MOTA	3594	C	GLN	142	28.915	8.984	40.473	1.00 12.11	В
	MOTA	3595	ō	GLN	142	28.206	8.585	39.560	1.00 11.87	В
	ATOM	3596	N	ILE	143	28.434	9.664	41.506	1.00 11.12	В
50	MOTA	3597	CA	ILE	143	27.018	10.010	41.573	1.00 12.39	В
	ATOM	3598	СВ	ILE	143	26.722	10.953	42.788	1.00 12.55	В
	ATOM	3599	CG2	ILE	143	25.341	11.608	42.650	1.00 12.75	В
	ATOM	3600	CG1	ILE	143	26.784	10.147	44.093	1.00 13.10	В
	MOTA	3601	CD1	ILE	143	26.532	10.971	45.338	1.00 10.72	В
55	MOTA	3602	C	ILE	143	26.587	10.710	40.275	1.00 13.82	В
	MOTA	3603	0	ILE	143	25.541	10.391	39.705	1.00 14.18	В
	ATOM	3604	N	PHE	144	27.397	11.666	39.816	1.00 14.48	В
	MOTA	3605	CA	PHE	144	27.099	12.430	38.605	1.00 15.02	В
60	MOTA	3606	CB	PHE	144	28.023	13.646	38.513	1.00 14.03	B B
60	MOTA	3607	CG	PHE	144	27.773	14.676	39.585	1.00 12.67	_
	ATOM	3608		PHE	144	26.680	15.527	39.510	1.00 10.36	B
	MOTA	3609		PHE	144	28.623	14.796	40.678	1.00 13.84	В
	MOTA	3610		PHE	144	26.442	16.473 15.761	41.680	1.00 9.69 1.00 13.70	В
65	MOTA	3611		PHE	144	28.375		41.578		В
UJ	MOTA	3612	CZ	PHE	144	27.286 27.223	16.591 11.586	37.348	1.00 16.57	В
	MOTA	3613	C	PHE	144	26.516	11.835	36.384	1.00 16.66	В
	ATOM	3614	0	PHE	144 145	28.123	10.593	37.364	1.00 20.10	В
	MOTA	3615 3616	N CA	GLU	145	28.335	9.691	36.210	1.00 22.03	В
70	MOTA MOTA	3617	CB	GLU	145	29.597	8.825	36.352	1.00 26.12	B
7.0	ATOM	3618	CG	GLU	145	30.902	9.538	36.044	1.00 32.68	В
	MOTA	3619	CD	GLU		31.004	9.949	34.595	1.00 36.87	В
	ATOM	3620		GLU		31.965	10.666	34.249	1.00 39.57	В
	0.,					-		_		

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	MOTA	3621	OE2	GLU	145	30.121	9.549	33.807	1.00 40.00	В
	ATOM	3622	С	GLU	145	27.194	8.705	36.029	1.00 21.04	В
	MOTA	3623	0	GLU	145	26.750	8.470	34.943	1.00 20.94	В
	ATOM	3624	N	LYS	146	26.728	8.129	37.127	1.00 22.01	В
5							7.166	37.072	1.00 22.94	В
9	MOTA	3625	CA	LYS	146	25.628				
	MOTA	3626	CB	LYS	146	25.489	6.433	38.423	1.00 24.69	В
	MOTA	3627	CG	LYS	146 -	26.725	5.599	38.799	1.00 27.30	В
	ATOM	3628	CD	LYS	146	26.480	4.519	39.854	1.00 24.53	В
	MOTA	3629	CE	LYS	146	27.560	3.447	39.715	1.00 25.61	В
10		3630		LYS	146	27.404	2.262	40.595	1.00 24.71	В
10	MOTA		NZ							В
	MOTA	3631	C	LYS	146	24.281	7.799	36.702	1.00 24.00	
	MOTA	3632	0	LYS	146	23.472	7.178	36.020	1.00 24.07	В
	MOTA	3633	N	LEU	147	24.049	9.035	37.138	1.00 23.75	В
	ATOM	3634	CA	LEU	147	22.788	9.720	36.850	1.00 24.08	В
15	ATOM	3635	CB	LEU	147	22.247	10.365	38.123	1.00 24.33	В
13					147		9.460	39.325	1.00 24.88	В
	ATOM	3636	CG	LEU		21.976				
	ATOM	3637		LEU	147	21.607	10.299	40.537	1.00 24.59	В
	MOTA	3638	CD2	LEU	147	20.847	8.493	39.014	1.00 24.04	В
	MOTA	3639	С	LEU	147	22.895	10.796	35.762	1.00 25.02	В
20	ATOM	3640	0	LEU	147	22.110	11.755	35.736	1.00 22.56	В
	ATOM	3641	N	THR	148	23.857	10.627	34.857	1.00 27.04	В
						24.073	11.585	33.774	1.00 28.40	В.
	MOTA	3642	CA	THR	148					В.
	MOTA	3643	CB	THR	148	25.296	11.194	32.905	1.00 28.80	
~ ~	MOTA	3644	OG1	THR	148	25.479	12.150	31.850	1.00 29.27	B
25	MOTA	3645	CG2	THR	148	25.108	9.794	32.318	.1.00 30.26	В
	MOTA	3646	С	THR	148	22.855	11.738	32.865	1.00 28.70	В
	ATOM	3647	ō	THR	148	22.466	12.848	32.580	1.00 29.54	В
		3648					10.638	32.413	1.00 27.95	В
	MOTA		N	ASP	149	22:253				В
20	ATOM	3649	CA	ASP	149	21.087	10.749	31.533	1.00 28.50	
30	MOTA	3650	CB	ASP	149	21.500	11.014	30.067	1.00 28.76	В
	ATOM	3651	CG	ASP	149	22.520	10.010	29.522	1.00 29.99	В
	MOTA	3652	OD1	ASP	149	22.501	8.830	29.939	1.00 29.75	В
	MOTA	3653		ASP	149	23.332	10.408	28.646	1.00 29.41	В
	ATOM					20.148	9.551	31.576	1.00 28.84	В
35		3654	C	ASP	149					В
22	MOTA	3655	0	ASP	149	19.636	9.096	30.555	1.00 27.84	
	MOTA	3656	N	asn	150	19.899	9.055	32.778	1.00 29.57	В
	MOTA	3657	CA	ASN	150	19.008	7.912	32.928	1.00 31.21	В
	ATOM	3658	CB	ASN	150	19.483	7.010	34.080	1.00 29.55	B
	ATOM	3659	CG	ASN	150	19.259	7.641	35.459	1.00 28.21	В
40		3660		ASN	150	19.347	8.859	35.618	1.00 27.26	В
40	MOTA									B
	ATOM	3661		ASN	150	18.969	6.804	36.458	1.00 25.05	
	MOTA	3662	С	ASN	150	17.550	8.345	33.175	1.00 31.80	В
	ATOM	3663	0	ASN	150	16.693	7.501	33.485	1.00 32.95	В
	ATOM	3664	N	GLY	151	17.279	9.648	33.043	1.00 30.56	В
45	ATOM	3665	CA	GLY	151	15.939	10.169	33.247	1.00 29.70	В
	ATOM	3666	c.	GLY	151	15.601	10.387	34.701	1.00 29.38	В
									1.00 29.95	В
	MOTA	3667	0	GLY	151	14.462	10.518	35.052		
	MOTA	3668	N	THR	152	16.616	10.412	35.549	1.00 29.90	В
	MOTA	3669	CA	THR	152	16.386	10.634	36.964	1.00 30.17	В
50	MOTA	3670	CB	THR	152	17.082	9.552	37.805	1.00 29.93	В
	MOTA	3671	OGI	THR	152	16.662	8.249	37.373	1.00 29.92	В
	ATOM	3672		THR	152	16.739	9.730	39.272	1.00 31.14	В
						16.902	12.022	37.384	1.00 31.11	В
	ATOM	3673	С	THR	152					В
55	MOTA	3674	0	THR	152	18.104	12.232	37.543	1.00 32.13	
55	MOTA	3675	N	GLU	153	15.977	12.968	37.531	1.00 30.29	В
	MOTA	3676	CA	GLU	153	16.310	14.325	37.948	1.00 28.58	В
	ATOM	3677	CB	GLU	153	15.041	15.174	37.977	1.00 31.74	В
	ATOM	3678	CG	GLU	153	15.257	16.669	37.853	1.00 35.57	В-
		3679	co	GLU	153	15.641	17.082	36.438	1.00 38.01	В
60	MOTA									
UU	MOTA	3680		GLU	153	15.923	18.281	36.200	1.00 38.59	В
	MOTA	3681	OE2	GLU	153	15.655	16.201		1.00 39.17	B
	MOTA	3682	С	GLU	153	16.861	14.173	39.366	1.00 25.90	В
	ATOM	3683	0	GLU	153	16.382	13.346	40.114	1.00 25.18	В
	ATOM	3684	N	PHE	154	17.852	14.978	39.738	1.00 24.45	В
65							14.852	41.074	1.00 21.39	В
00	MOTA	3685	CA	PHE	154	18.447				
	MOTA	3686	CB	PHE	154	19.411	13.651	41.115	1.00 20.65	В
	MOTA	3687	CG	PHE	154	20.679	13.846	40.306	1.00 20.31	В
	ATOM	3688	CD1	PHE	154	21.853	14.284	40.904	1.00 19.86	В
	ATOM	3689		PHE	154	20.698	13.570	38.945	1.00 19.64	В
70	ATOM	3690		PHE	154	23.021	14.435	40.142	1.00 21.56	В
				PHE	154	21.856	13.720	38.194	1.00 20.70	В
	MOTA	3691								В
	MOTA	3692	CZ	PHE	154	23.017	14.149	38.786	1.00 19.85	
	MOTA	3693	¢	PHE	154	19.224	16.073	41.567	1.00 19.03	В

	MOTA	3694	0	PHE	154	19.579	16.970	40.805	1.00 18.07	В
	MOTA	3695	N	SER	155	19.470	16.107	42.865	1.00 17.25	В
	ATOM	3696	CA	SER	155	20.234	17.200	43.451	1.00 17.56	В
		3697	CB	SER	155	19.310	18.302	44.043	1.00 18.40	В
5	MOTA			SER	155	18.744	17.999	45.315	1.00 19.07	В
)	MOTA	3698	OG			21.072	16.536	44.521	1.00 16.97	В
	MOTA	3699	C	SER	155				1.00 15.32	В
	MOTA	3700	0	SER	155	20.629	15.587	45.157	1.00 17.21	В
	MOTA	3701	N	VAL	156	22.286	17.034	44.708		В
	MOTA	3702	CA	VAL	156	23.181	16.479	45.709	1.00`15.73	
10	MOTA	3703	CB	VAL	156	24.452	15.964	45.066	1.00 16.35	В
	MOTA	3704	CG1	VAL	156	25.307	15.319	46.089	1.00 16.70	В
	MOTA	3705	CG2	VAL	156	24.117	14.993	43.973	1.00 18.36	· В
	MOTA	3706	С	VAL	156	23.577	17.503	46.762	1.00 14.63	В
	MOTA	3707	0	VAL	156	24.031	18.595	46.441	1.00 12.84	В
15	ATOM	3708	N	LYS	157	23.394	17.138	48.024	1.00 15.08	В
	ATOM	3709	CA	LYS	157	23.739	18.019	49.139	1.00 16.33	В
	MOTA	3710	CB	LYS	157	22.485	18.370	49.962	1.00 17.27	В
	MOTA	3711	CG	LYS	157	21.640	19.492	49.381	1.00 19.38	В
	MOTA	3712	CD	LYS	157	20.323	19.704	50.121	1.00 19.23	В
20		3713	CE	LYS	157 .	19.563	20.911	49.535	1.00 20.48	В
20	MOTA			LYS	157	20.216	22.239	49.815	1.00 19.89	В
	MOTA	3714	NZ			24.738	17.288	50.025	1.00 15.63	В
	MOTA	3715	C	LYS	157		16.118	50.305	1.00 17.71	В
	MOTA	3716	0	LYS	157	24.568		50.447	1.00 14.09	В
25	MOTA	3717	N	VAL	158	25.789	17.979	51.313		В
25	MOTA	3718	CA	VAL	158	26.782	17.350		1.00 12.31	В
	MOTA	3719	СВ	VAL	158	28.184	17.314	50.670	1.00 12.25	В
	MOTA	3720	CG1	VAL	158	28.150	16.490	49.405		В
	MOTA	3721	CG2	VAL	158	28.657	18.731	50.367	1.00 11.55	В
20	MOTA	3722	Ç	VAL	158	26.911	18.070	52.636	1.00 11.94	В
30	MOTA	3723	0	VAL	158	26.668	19.270	52.726	1.00 11.97	
	MOTA	3724	N	SER	159	27.301	17.321	53.659	1.00 10.91	В
-	MOTA	3725	CA	SER	159	27.490	17.876	54.992	1.00 11.22	В
	MOTA	3726	CB	SER	159	26.245	17.662	55.846	1.00 11.02	В
~~	ATOM	3727	OG	SER	159	25.184	18.476	55.385	1.00 17.68	В
35	ATOM	3728	С	SER	159	28.677	17.212	55.667	1.00 11.18	В
	MOTA	3729	0	SER	159	28.925	16.002	55.499	1.00 10.26	В
	MOTA	3730	N	LEU	160	29.431	18.011	56.405	1.00 11.19	В
	MOTA	3731	CA	LEU	. 160	30.583	17.495	57.115	1.00 11.64	В
	MOTA	3732	CB	LEU	160	31.875	18.043	56.498	1.00 11.99	В
40	MOTA	3733	CG	LEU	160	33.168	17.440	57.061	1.00 12.29	В
	MOTA	3734	CD1	LEU	160	33.088	15.915	57.170	1.00 12.16	В
	MOTA	3735	CD2	LEU	160	34.307	17.848	56.170	1.00 13.02	В
	MOTA	3736	С	LEU	160	30.476	17.836	58.606	1.00 12.31	В
	MOTA	3737	0	LEU	160	30.894	18.913	59.056	1.00 13.72	В
45	MOTA	3738	N	LEU	161	29.921	16.899	59.365	1.00 11.68	В
	MOTA	3739	CA	LEU	. 161	29.728	17.056	60.794	1.00 11.73	В
	MOTA	3740	CB	LEU	161	28.387	16.462	61.184	1.00 10.86	В
	MOTA	3741	CG	LEU	161	28.069	16.373	62.667	1.00 11.21	В
	MOTA	3742	CD1	LEU	161	28.038	17.772	63.257	1.00 14.64	В
50	MOTA	3743	CD2	LEU	161	26.735	15.687	62.849	1.00 11.87	В
	ATOM	3744	С	LEU	161	30.805	16.318	61.565	1.00 11.76	В
	ATOM	3745	0	LEU	161	31.023	15.148	61.353	1.00 14.92	В
	MOTA	3746	N	GLU	162	31.493	17.005	62.461	1.00 11.26	В
	MOTA	3747	CA	GLU	162 .	32.536	16.335	63.230	1.00 10:12	В
55	ATOM	3748	CB	GLU	162 .	33.914	16.845	62.829	1.00 9.47	В
	ATOM	3749	CG	GLU	162	34.143	16.845	61.353	1.00 9.35	В
	ATOM	3750	CD	GLU	162	35.607	16.813	61.008	1.00 9.38	В
	ATOM	3751	OE1		162	36.443	17.239	61.829	1.00 9.19	В
	MOTA	3752		GLU	162	35.929	16.357	59.901	1.00 8.99	В
60	MOTA	3753	C	GLU	162	32.339	16.498	64.729	1.00 10.38	В
00					162	31.849	17.527	65.222	1.00 7.96	В
	MOTA	3754	0	GLU		32.734	15.456	65.444	1.00 10.66	В
	MOTA	3755	N	ILE	163	32.581	15.414	66.879	1.00 10.98	В
	MOTA	3756	CA	ILE	163				1.00 11.27	В
65	MOTA	3757	CB	ILE	163	31.782	14.160	67.293	1.00 11.27	В
ŲĴ	MOTA	3758		ILE	163	31.505	14.192	68.793		В
	MOTA	3759		ILE	163	30.504	14.066	66.462	1.00 11.37	В
	ATOM	3760		ILE	163	29.804	12.728	66.528	1.00 12.73	
	MOTA	3761	C	ILE	163	33.941	15.387	67.559	1.00 10.94	В
70	MOTA	3762	0	ILE	163	34.849	14.680	67.127	1.00 11.24	В
70	MOTA	3763	N	TYR	164	34.071	16.177	68.619	1.00 10.16	В
	ATOM	3764	CA	TYR	164	35.303	16.245	69.376	1.00 8.14	В
	ATOM	3765	CB	TYR	164	36.254	17.270	68.759	1.00 5.82	В
	MOTA	3766	CC	TYR	164	37.517	17.425	69.533	1.00 3.86	В

					364	37 560		70 (00	1 00 5 60	
	MOTA	3767		TYR	164	37.560	18:215	70.682	1.00 5.62	В
	ATOM	3768		TYR	164	38.709	18.292	71.465	1.00 4.56	В
	MOTA	3769	CD2	TYR	164	38.651	16.719	69.177	1.00 3.71	В
-	MOTA	3770	CE2	TYR	164	39.811	16.786	69.955	1.00 5.19	В
5	MOTA	3771	CZ	TYR	164	39.827	17.577	71.094	1.00 4.77	В
	MOTA	3772	ОН	TYR	164	40.976	17.675	71.832	1.00 5.42	В
	MOTA	3773	С	TYR	164	34.937	16.617	70.802	1.00 8.94	В
	MOTA	3774	0	TYR	164	34.299	17.627	71.061	1.00 9.91	В
	MOTA	3775	N	ASN	165	35.346	15.775	71.731	1.00 10.87	B
10	ATOM	3776	CA	ASN	165	35.050	16.003	73.134	1.00 12.54	В
	ATOM	3777	CB	ASN	165	35.847	17.192	73.674	1.00 15.11	В
	MOTA	3778	CG	ASN	165	35.722	17.336	75.190	1.00 19.28	В
	MOTA	3779		ASN	165	35.971	16.385	75.936	1.00 21.80	В
	ATOM	3780		ASN	165	35.345	18.528	75.651	1.00 20.20	В
15	ATOM	3781	c	ASN	165	33.562	16.262	73.308	1.00 12.20	В
	MOTA	3782	ŏ	ASN	165	33.160	17.158	74.000	1.00 10.80	В
	ATOM	3783	N	GLU	166	32.767	15.430	72.646	1.00 16.33	В
	ATOM	3784	CA	GLU	166	31.304	15.495	72.656	1.00 18.28	В
	ATOM	3785	CB	GLU	166	30.739	15.101	74.031	1.00 17.10	В
20	ATOM	3786	CG	GLU	166	30.887	13.610	74.353	1.00 16.82	В
20	ATOM	3787	CD	GLU	166	30.175	12.693	73.357	1.00 16.06	В
	ATOM	3788		GLU	166	28.928	12.606	73.360	1.00 13.96	В.
		3789		GLU	166	30.880	12.055	72.559	1.00 15.35	В.
	ATOM							72.201	1.00 19.60	В
25	ATOM	3790	Č	GLU	166	30.697	16.825			В
43	MOTA	3791	0	GLU	166	29.604	17.192	72.606	1.00 19.36	
	ATOM	3792	N	GLU	167	31.427	17.546	71.357	1.00 21.89	В
	MOTA	3793	Cλ	GLU	167	30.956	18.818	70.823	1.00 22.41	В
	ATOM	3794	CB	GLU	167	31.910	19.947	71.208	1.00 24.57	В
20	MOTA	3795	CG	GLU	167	31.998	20.181	72.701	1.00 28.83	В
30	MOTA	3796	CD	CLU	167	32.847	21.376	73.044	1.00 31.70	В
	MOTA	3797		GLU	167	33.985	21.472	72.521	1.00 32.58	В
	MOTA	3798		GLU	167	32.373	22.214	73.840	1.00 33.47	В
	ATOM	3799	С	GLU	167	30.874	18.683	69.314	1.00 21.24	В
25	MOTA	3800	0	GLU	167	31.689	17.997	68.700	1.00 20.64	В
35	MOTA	.3801	N	LEU	168	29.879	19.328	68.717	1.00 20.17	В
	MOTA	3802	CA	LEU	168	29.712	19.254	67.269	1.00 19.71	В
	MOTA	3803	CB	LEU	168	28.240	19.110	66.887	1.00 19.82	В
	ATOM	3804	CG	LEU	168	27.430	17.954	67.457	1.00 19.46	В
	MOTA	3805	CD1	LEU	168	28.198	16.653	67.320	1.00 19.39	В
40	MOTA	3806	CD2	·LEU	168	27.113	18.236	68.903	1.00 20.70	В
	MOTA	3807	С	LEU	168	30.251	20.477	66.524	1.00 19.80	В
	MOTA.	3808	٥	LEU	168	30.055	21.611	66.939	1.00 20.40	В
	MOTA	3809	N	PHE	169	30.928	20.229	65.411	1.00 19.38	В
	ATOM	3810	CA	PHE	169	31.478	21.306	64.612	1.00 17.82	В
45	MOTA	3811	CB	PHE	169	33.004	21.327	64.706	1.00 17.88	В
_	ATOM	3812	CG	PHE	169	33.513	21.530	66.097	1.00 16.09	В
	MOTA	3813		PHE	169	33.737	20.445	66.928	1.00 15.76	В
	MOTA	3814		PHE	. 169	33.695	22.810	66.600	1.00 16.92	В
	MOTA	3815		PHE	169	34.130	20.621	68.235	1.00 16.10	В
50	MOTA	3816		PHE	169	34.090	23.001	67.907	1.00 17.09	В
	MOTA	3817	cz	PHE	169	34.308	21.901	68.731	1.00 16.73	В
	MOTA	3818	c	PHE	169	31.068	21.102	63.166	1.00 18.77	. B
	ATOM	3819	ŏ	PHE	169	30.929	19.980	62.704	1.00 18.62	. B
	MOTA	3820	N	ASP	170	30.871	22.206	62.459	1.00 20.24	В
55	ATOM	3821	CA	ASP	170	30.476	22.171	61.055	1.00 21.83	В
55	ATOM	3822	CB	ASP	170	29.387	23.216	60.785	1.00 20.71	В
								59.382	1.00 22.77	В
	MOTA	3823	CG	ASP	170	28.832	23.135			В.
	MOTA	3824		ASP	170	29.510	22.563	58.493	1.00 23.50	
60	MOTA	3825		ASP	170	27.724	23.658	59.158	1.00 24.44	В
UU	MOTA	3826	С	ASP	170	31.714	22.545	60.269	1.00 22.03	В
	MOTA	3827	0	ASP	170	32.119	23.693	60.281	1.00 23.16	В
	MOTA	3828	N	LEU	171	32.320	21.577	59.593	1.00 21.95	В
	MOTA	3829	CA	LEU	171	33.514	21.878	.58.828	1.00 22.12	В
66	MOTA	3830	СB	LEU	171	34.449	20.674	58.827	1.00 20.38	В
65	MOTA	3831	CG	LEU	171	35.422	20.605	60.013	1.00 21.16	В.
	MOTA	3832		LEU	171	36.359	21.824	60.018	1.00 20.44	В
	MOTA	3833	CD2	LEU	171	34.645	20.544	61.307	1.00 18.78	В
	MOTA	3834	С	LEU	171	33.271	22.356	57.402	1.00 24.20	В
	MOTA	3835	0	LEU	171	34.201	22.357	56.582	1.00 24.74	В
70	MOTA	3836	N	LEU	172	32.034	22.764	57.108	1.00 26.40	В
	ATOM	3837	CA	LEU	172	31.686	23.266	55.776	1.00 28.39	B
	ATOM	3838	CB	LEU	172	30.802	22.283	55.004	1.00 28.49	B
	MOTA	3839	CG	LEU	172	31.536	21.056	54.448	1.00 29.54	В

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	MOTA	3840		LEU	172	30.562	20.216	53.633	1.00 30.71	В
	MOTA	3841	CD2	LEU	172	32.730	21.477	53.583	1.00 28.53	В
	ATOM	3842	С	LEU	172	30.979	24.607	55.797	1.00 28.89	В
	MOTA	3843	0	LEU	172	30.416	25.030	54.823	1.00 30.09	₿
5	MOTA	3844	N	ASN	173	31.007	25.264	56.941	1.00 31.10	B
•	ATOM	3845	CA	ASN	173	30.403	26.580	57.043	1.00 34.00	В
									1.00 33.23	В
	MOTA	3846	CB	ASN	173	29.606	26.708	58.347		
	MOTA	3847	ÇG	ASN	173	28.903	28.053	58.473	1.00 32.72	В
	ATOM	3848	OD1	ASN	173	28.108	28.268	59.381	1.00 33.30	В
10	MOTA	3849	ND2	ASN	173	29.205	28.967	57.551	1.00 31.17	B
	MOTA	3850	С	ASN	173	31.554	27.579	56.982	1.00 35.93	Ð
	ATOM	3851	ō	ASN	173	32.402	27.627	57.861	1.00 35.47	В
				PRO		31.609	28.372	55.908	1.00 38.25	В
	MOTA	3852	N		174					
15	MOTA	3853	CD	PRO	174	30.799	28.283	54.6B1	1.00 38.57	В
15	MOTA	3854	CA	PRO	174	32.674	29.362	55.753	1.00 40.38	B
	MOTA	3855	CB	PRO	174	32.702	29.569	54.242	1.00 39.65	В
	MOTA	3856	CG	PRO	174	31.264	29.478	53.900	1.00 38.79	В
	MOTA	3857	С	PRO	174	32.445	30.632	56.582	1.00 42.95	В
	MOTA	3858	ō	PRO	174	33:356	31.450	56.743	1.00 43.55	В
20	ATOM	3859	N	SER	175	31.234	30.794	57.108	1.00 45.10	В
20									1.00 47.15	В
	MOTA	3860	CA	SER	175	30.906	31.974	57.913		
	MOTA	3861	CB	SER	175	29.395	32.227	57.889	1.00 47.30	В
	MOTA	3862	OG	SER	175	28.906	32.331	56.559	1.00 49.37	В
	ATOM	3863	С	SER	175	31.369	31.882	59.376	1.00 47.57	В
25	MOTA	3864	0	SER	175	31.800	32.872	59.970	1.00 48.25	В
	ATOM	3865	N	SER	176	31.280	30.690	59.953	1.00 47.97	В
	MOTA	3866	CA	SER	176	31.677	30.487	61.340	1.00 47.64	В
								62.034	1.00 46.90	В
	MOTA	3867	CB	SER	176	30.720	29.520			
20	MOTA	3868	OG	SER	176	30.794	28.230	61.447	1.00 46.36	В
30	MOTA	3869	С	SER	176	33.083	29.917	61.451	1.00 48.54	В
	ATOM	3870	0	SER	176	33.650	29.434	60.484	1.00 48.78	В
	MOTA	3871	N	ASP	177	33.646	29.989	62.64B	1.00 49.43	В
	ATOM	3872	CA	ASP	177	34.979	29.467	62.874	1.00 50.07	В
	ATOM	3873	CB	ASP	177	35.843	30.521	63.591	1.00 51.58	В
35						35.342	30.852	64.996	1.00 53.37	В
33	MOTA	3874	CG	ASP	177					
	MOTA	3875		ASP	177	35.948	31.723	65.658	1.00 54.70	В
	MOTA	3876	OD2	ASP	177	34.353	30.246	65.452	1.00 54.61	В
	MOTA	3877	С	ASP	177	34.880	28.160	63.669	1.00 49.81	В
	ATOM	3878	0	ASP	177	33.833	27.830	64.235	1.00 48.89	В
40	MOTA	3879	N	VAL	178	35.980	27.422	63.707	1.00 49.42	В
	ATOM	3880	CA	VAL	178	36.030	26.146	64.409	1.00 50.03	В
	ATOM	3881	CB	VAL	178	37.385	25.452	64.150	1.00 50.76	В
										В
	MOTA	3882		VAL	178	37.528	25.131	62.665	1.00 49.77	
4.5	MOTA	3883		VAL	178	38.538	26.353	64.629	1.00 50.93	В
45	MOTA	3884	C	VAL	178	35.791	26.203	65.927	1.00 49.82	В
	ATOM	3885	0	VAL	178	35.912	25.194	66.623	1.00 50.17	В
	MOTA	3886	N	SER	179	35.451	27.372	66.447	1.00 48.85	В
	MOTA	3887	CA	SER	179	35.225	27.491	67.877	1.00 47.91	В
	MOTA	3888	СВ	SER	179	35.912	28.749	68.397	1.00 48.14	В
50							29.884	67.667	1.00 47.90	В
50	ATOM	3889	0G	SER	179	35.472				
	MOTA	3890	С	SER	179	33.739	27.541	68.211	1.00 47.46	В
	MOTA	3891	0	SER	179	33.357	27.618	69.376	1.00 47.10	В
	ATOM	3892	N	GLU	180	32.900	27.495	67.182	1.00 46.50	В
	ATOM	3893	CA	GLU	180	31.458	27.542	67.383	1.00 45.18	В
55	MOTA	3894	CB	GLU	180	30.835	28.527	66.383	1.00 44.47	В
	MOTA	3895	ÇG	GLU	180	31.026	29.983	66.788	1.00 44.05	В
				GLU	180		30.971	65.724	1.00 43.63	В
	ATOM	3896	CD			30.595				
	MOTA	3897		GLU	180	31.354	31.176	64.751	1.00 43.67	В
C O	MOTA	3898		GLU	180	29.495	31.542	65.860	1.00 42.55	В
60	MOTA	3899	С	GLU	180	30.813	26.156	67.295	1.00 44.60	В
	ATOM	3900	0	GLU	180	30.714	25.570	66.228	1.00 44.37	В
	ATOM	3901	N	ARG	181	30.373	25.650	68.445	1.00 44.01	В
	MOTA	3902	CA	ARG	181	29.739	24.342	68.529	1.00 42.83	В
									1.00 45.18	
65	ATOM	3903	CB	ARG	181	29.775	23.806	69.958		В
65	MOTA	3904	CC	ARG	181	28.755	24.439	70.895	1.00 47.37	В
	MOTA	3905	CD	ARG	181	28.693	23.644	72.187	1.00 51.45	В
	MOTA	3906	NE	ARG	181	27.541	23.972	73.034	1.00 54.79	В
	MOTA	3907	CZ	ARG	181	26.267	23.753	72.706	1.00 56.32	В
	MOTA	3908		ARG	181	25.969	23.205	71.539	1.00 57.53	В
70									1.00 56.18	В
,,,	ATOM	3909	NH2	ARG	181	25.286	24.065	73.548		
	MOTA	3910	C	ARG	181	28.278	24.404	68.121	1.00 40.59	В
	MOTA	3911	0.	ARG	181	27.632	25.414	68.254	1.00 41.20	В
	ATOM	3912	N	LEU	182	27.759	23.293	67.632	1.00 38.61	В

	ATOM	3913	CA	LEU	182	26.370	23.253	67.219	1.00 35.94	B
	ATOM	3914	CB	LEU	182	26.259	22.490	65.897	1.00 34.47	В
	ATOM	3915	CG	LEU	182	27.018	23.098	64.718	1.00 31.55	В
	ATOM	3916		LEU	182	26.951	22.179	63.525	1.00 30.32	В
5										
,	ATOM	3917		LEU	182	26.417	24.440	64.382	1.00 29.89	В
	MOTA	3918	С	LEU	182	25.532	22.579	68.300	1.00 35.46	В
	MOTA	3919	0	LEU	182	26.057	21.845	69.139	1.00 35.35	В
	MOTA	3920	N	GLN	183	24.227	22.839	68.270	1.00 35.14	В
	ATOM	3921	CA	GLN	183	23.290	22.256	69.228	1.00 33.43	В
10	MOTA	3922	CB	GLN	183	22.261	23.284	69.688	1.00 36.19	В
10										
	ATOM	3923	·CG	GLN	183	22.844	24.463	70.456	1.00 40.60	В
	ATOM	3924	CD	GLN	183	21.781	25.458	70.916	1.00 43.17	В
	MOTA	3925	OE1	GLN	183	20.902	25.122	71.711	1.00 45.10	В
	ATOM	3926	NE2	GLN	183	21.856	26.687	70.408	1.00 42.17	В
15	ATOM	3927	С	GLN	183	22.513	21.122	68.578	1.00 30.84	В
	ATOM	3928	ŏ	GLN	183	22.098	21.224	67.436	1.00 29.43	В
	MOTA	3929		MET	184	22.311	20.047	69.325	1.00 29.11	В
			N							
	MOTA	3930	CA	MET	184	21 - 603	18.884	68.821	1.00 28.51	В
20	MOTA	3931	CB	MET	184	22.549	17.698	68.930	1.00 27.68	В
20	ATOM	3932	CG	MET	184	21.997	16.385	68.443	1.00 30.34	В
	ATOM	3933	SD	MET	184	23.142	15.021	68.745	1.00 30.67	В
	ATOM	3934	CE	MET	184	22.841	14.793	70.448	1.00 30.06	В.
	ATOM	3935	c	MET	184	20.298	18.650	69.595	1.00 29.09	В
									1.00 29.05	·B
25	MOTA	3936	0	MET	184	20.280	18.737	70.806		
23	MOTA	3937	N	PHE	185	19.213	18.342	68.887	1.00 30.68	В
	MOTA	3938	CA	PHE	185	17.921	18.112	69.537	1.00 31.83	В
	MOTA	3939	CB	PHE	185	16.953	19.277	69.291	1.00 31.45	В
	MOTA	3940	CG	PHE	185	17:520	20.626	69.637	1.00 30.24	В
	ATOM	3941	CD1	PHE	185	18.381	21.275	68.763	1.00 29.12	В
30	MOTA	3942		PHE	185	17.215	21.234	70.850	1.00 28.98	В
50	MOTA	3943		PHE	185	18.929	22.500	69.082	1.00 28.97	В
	MOTA	3944		PHE	185	17.762	22.461	71.180	1.00 29.87	В.
	MOTA	3945	CZ	PHE	185	18.624	23.098	70.289	1.00 29.79	B
~	ATOM	3946	С	PHE	185	17.236	16.883	68.976	1.00 33.71	В
35	MOTA	3947	0	PHE	185	· 17.473	16.515	67.845	1.00 33.43	В
	MOTA	3948	N	ASP	186	16.393	16.245	69.782	1.00 37.53	В
	ATOM	3949	CA	ASP	186	15.667	15.071	69.310	1.00 40.98	В
	ATOM	3950	CB	ASP	186	14.857	14.413	70.431	1.00 43.17	В
40	MOTA	3951	CG	ASP	186	15.721	13.931	71.575	1.00 45.72	В
40	MOTA	3952		ASP	186	16.691	13.190	71.316	1.00 48.29	В
	ATOM	3953	OD2	ASP	186	15.413	14.291	72.734	1.00 46.64	В
	ATOM	3954	С	ASP	186	14.676	15.587	68.284	1.00 42.58	В
	ATOM	3955	0	ASP	186	14.123	16.666	68.453	1.00 42.55	В
	ATOM	3956	N	ASP	187	14.457	14.835	67.214	1.00 44.89	В
45	ATOM	3957	CA	ASP	.187	13.528	15.287	66.188	1.00 46.96	В
1.5								64.840	1.00 46.56	В
	MOTA	3958	CB	ASP	187	13.921	14.695			
	MOTA	3959	CC	ASP	187	13.090	15.232	63.718	1.00 46.68	В
	ATOM	3960	OD1	ASP	187	13.381	14.891	62.555	1.00 47.95	В
	ATOM	3961	OD2	ASP	187	12.144	15.996	64.008	1.00 45.37	В
50	MOTA	3962	С	ASP	187	12.127	14.881	66.604	1.00 48.78	Ð
	MOTA	3963	0	ASP	187	11.844	13.696	66.773	1.00 49.04	В
	MOTA	3964	N	PRO	188	11.235	15.870	66.799	1.00 50.85	В
	ATOM	3965	CD		188	11.546	17.310	66.716	1.00 50.78	В
				PRO						
55	MOTA	3966	CA	PRO	188	9.838	15.660	67.209	1.00 52.07	В
55	MOTA	3967	CB	PRO	188	9.280	17.085	67.240	1.00 51.41	В
	ATOM	3968	CG	PRO	188	10.496	17.916	67.605	1.00 50.84	В
	MOTA	3969	С	PRO	188	9.071	14.705	66.302	1.00 53.79	В
	MOTA	3970	o	PRO	188	8.249	13.900	66.753	1.00 52.56	В
	ATOM	3971	N	ARG	189	9.340	14.817	65.011	1.00 56.26	В
60										В
vv	MOTA	3972	CA	ARG	189	8.691	13.979	64.033	1.00 59.28	_
	MOTA	3973	CB	ARG	189	9.218	14.349	62.649	1.00 60.03	В
	MOTA	3974	CG	ARG	189	8.875	15.774	62.238	1.00 61.54	В
	MOTA	3975	CD	ARG	189	9.366	16.081	.60.833	1.00 62.62	В
	ATOM	3976	NE	ARG	189	10.813	16.277	60.790	1.00 63.59	В
65	ATOM	3977	CZ	ARG	189	11.407	17.465	60.B37	1.00 64.36	В
	ATOM	3978	NH1				18.575	60.925	1.00 64.67	В
					189	10.680				
	MOTA	3979	NH2		189	12.729	17.545	60.794	1.00 64.73	В
	MOTA	3980	С	ARG	189	8.905	12.499	64.357	1.00 61.00	В
70	MOTA	3981	0	ARG	189	7.952	11.725	64.399	1.00 61.27	В
70	MOTA	3982	N	ASN	190	10.159	12.118	64.590	1.00 63.40	В
	MOTA	3983	CA	ASN	190	10.516	10.735	64.914	1.00 65.21	В
	MOTA	3984	СВ	ASN	190	10.752	9.935	63.625	1.00 65.05	В
			CG				10.604		1.00 64.67	B
	MOTA	3985	CG	ASN	190	11.750	10.004	62.692	1.00 04.07	J

						40.054				_
	MOTA	3986		ASN	190	12.954	10.474	62.861	1.00 64.77	В
	MOTA	3987	ND2	ASN	190	11.242	11.332	61.707	1.00 63.52	В
	MOTA	3988	С	asn	190	11.757	10.684	65.807	1.00 66.41	В
	ATOM	3989	0	ASN	190	12.850	11.038	65.381	1.00 66.57	В
5	ATOM	3990	N	LYS	191	11.575	10.241	67.051	1.00 67.89	В
-					191	12.676	10.158	68.017	1.00 68.02	В
	MOTA	3991	CA	LYS						
	MOTA	3992	CB	LYS	191	12.151	9.687	69.378	1.00 69.77	В
	MOTA	3993	CG	LYS	191	11.151	10.636	70.012	1.00 71.09	В
	MOTA	3994	CD	LYS	191	11.787	11.982	70.297	1.00 72.77	В
10	MOTA	3995	CE	LYS	191	10.771	12.963	70.860	1.00 74.00	В
	MOTA	3996	NZ	LYS	191	9.657	13.210	69.902	1.00 75.27	В
					191	13.826	9.251	67.571	1.00 66.64	В
	MOTA	3997	C	LYS						
	MOTA	3998	0	LYS	191	14.852	9.149	68.253	1.00 66.18	В
	MOTA	3999	N	ARG	192	13.641	8.587	66.434	1.00 64.41	В
15	MOTA	4000	CA	ARG	192	14.668	7.720	65.878	1.00 62.32	В
	ATOM	4001	CB	ARG	192	14.101	6.946	64.685	1.00 64.84	В
	ATOM	4002	CG	ARG	192	15.134	6.138	63.909	1.00 68.49	В
					192	14.582	5.584	62.578	1.00 71.52	В
	MOTA	4003	CD	ARG						
20	MOTA	4004	NE	ARG	192	14.312	6.616	61.569	1.00 73.79	В
20	MOTA	4005	CZ	ARG	192	13.207	7.359	61.506	1.00 74.82	B
	MOTA	4006	NH1	ARG	192	12.232	7.201	62.393	1.00 75.36	В
	ATOM	4007	NH2	ARG	192	13.079	8.275	60.555	1.00 75.53	В
	ATOM	4008	C	ARG	192	15.822	8.612	65.403	1.00 59.33	В
	ATOM	4009	ŏ	ARG	192	16.991	8.235	65.479	1.00 58.48	В
25										В
23	MOTA	4010	N	GLY	193	15.468	9.805	64.927	1.00 55.93	
	MOTA	4011	CA	GLY	193	16.453	10.747	64.429	1.00 50.05	В
	MOTA	4012	С	GLY	193	16.778	11.895	65.364	1.00 45.96	В
	MOTA	4013	0	GLY	193	16.345	11.933	66.518	1.00 44.90	В
	MOTA	4014	N	VAL	194	17.547	12.842	64.839	1.00 42.75	В
30	MOTA	4015	CA	VAL	194	17.968	14.006	65.596	1.00 39.18	В
50							13.743	66.269	1.00 39.02	В
	MOTA	4016	CB	VAL	194	19.328				
	MOTA	4017		VAL	194	20.450	13.925	65.262	1.00 38.70	В
	ATOM	4018	CG2	VAL	194	19.504	.14.653	67.456	1.00 38.46	В
	MOTA	4019	С	VAL	194	18.096	15.209	64.666	1.00 37.27	В
35	ATOM	4020	0	VAL	194	18.181	15.057	63.456	1.00 36.48	В
	ATOM	4021	N	ILE	195	18.108	16.400	65.254	1.00 35.15	В
	MOTA	4022	CA	ILE	195	18.230	17.645	64.501	1.00 33.17	В
						17.002			1.00 34.99	В
	MOTA	4023	CB	ILE	195		18.543	64.702		
40	MOTA	4024		ILE	195	17.185	19.842	63.916	1.00 36.47	В
40	MOTA	4025	CG1	ILE	195	15.731	17.803	64.280	1.00 36.88	В
	MOTA	4026	CD1	ILE	195	15.658	17.513	62.784	1.00 38.32	В
	MOTA	4027	С	ILE	195	19.452	18.465	64.917	1.00 30.37	В
	MOTA	4028	0	ILE	195	19.575	18.870	66.063	1.00 28.47	В
	MOTA	4029	N	ILE	196	20.353	18.711	63.975	1.00 28.58	В
45								64.270	1.00 27.51	В
73	ATOM	4030	CA	ILE	196	21.538	19.503			
	MOTA	4031	CB	ILE	196	22.810	-18.928	63.572	1.00 26.71	В
	MOTA	4032	CG2	ILE	196	24.024	19.795	63.884	1.00 25.48	В
	MOTA	4033	CG1	ILE	196	23.107	17.515	64.078	1.00 25.19	В
	MOTA	4034	CD1	ILE	196	22.263	16.456	63.472	1.00 25.37	В
50	MOTA	4035	C	ILE	196	21.284	20.931	63.787	1.00 27.55	В
	MOTA	4036	ō	ILE	196	21.307	21.212	62.601	1.00 27.49	В
								64.730	1.00 28.27	В
	MOTA	4037	N	LYS	197	21.045	21.832			
	MOTA	4038	CA	LYS	197	20.765	23.229	64.418	1.00 27.24	В
	ATOM	4039	CB	LYS	197	20.328	23.973	65.688	1.00 28.18	В
55	ATOM	4040	CG	LYS	197	19.970	25.451	65.508	1.00 26.93	В
	MOTA	4041	CD	LYS	197	19.665	26.075	66.853	1.00 27.21	В
	MOTA	4042	CE	LYS	197	19.417	27.563	66.750	1.00 26.28	В
		4043		LYS	197	19.153	28.144	68.104	1.00 26.63	В
	MOTA		NZ							В
6 0	MOTA	4044	С	LYS	197	21.961	23.947	63.821	1.00 26.61	
60	MOTA	4045	0	LYS	197	23.039	23.974	64.406	1.00 27.65	В
	ATOM	4046	N	GLY	198	21.762	24.513	62.637	1.00 26.31	В
	ATOM	4047	CA	GLY	198	22.826	25.266	61.998	1.00 25.56	В
	ATOM	4048	c	GLY	198	23.747	24.536	61.044	1.00 24.60	В
	ATOM	4049	ō	GLY	198	24.518	25.162	60.335	1.00 24.69	В
65								61.029		B
UJ	ATOM	4050	N	LEU	199	23.680	23.211			
	MOTA	4051	CA	LEU	199	24.523	22.433	60.130	1.00 25.50	В
	MOTA	4052	CB	LEU	199	24.357	20.927	60.411	1.00 24.64	В
	MOTA	4053	CG	LEU	199	25.219	19.950	59.597	1.00 24.37	В
	ATOM	4054		LEU	199	26.699	20.274	59.742	1.00 22.90	В
70	ATOM	4055		LEU	199	24.942	18.535	60.068	1.00 23.77	В
	MOTA	4056	c	LEU	199	24.235	22.767	58.648	1.00 25.50	В
									1.00 24.77	В
	MOTA	4057	0	LEU	199	23.160	22.510	58.114		
	MOTA	4058	N	GLU	200	25.225	23.350	57.991	1.00 26.00	В

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	MOTA	4059	CA	GLU	200	25.087	23.722	56.598	1.00 26.47	В
	ATOM	4060	CB	GLU	200	26.274	24.568	56.143	1.00 27.75	В
	ATOM	4061	CG	GLU	200	26.324	25.971	56.724	1.00 32.47	В
	ATOM	4062	CD	GLU	200	25.112	26.821	56.339	1.00 35.25	В
5								57.004		В
J	ATOM	- 4063		GLU	200	24.061	26.700		1.00 38.07	
	MOTA	4064	OE2	GLU	200	25.196	27.600	55.363	1.00 35.41	В
	MOTA	4065	С	GLU	200	25.029	22.508	55.686	1.00 27.12	В
	ATOM	4066	0	GLU	200	25.586	21.457	55.972	1.00 26.69	В
	ATOM	4067	N	GLU	201	24.327	22.678	54.579	1.00 27.51	В
10	MOTA	4068	CA	GLU	201	24.218	21.646	53.574	1.00 26.72	В
10			CB		201	22.790	21.135	53.468	1.00 27.33	В
	ATOM .	4069		GLU						В
	ATOM	4070	CG	GLU	201	22.239	20.532	54.722	1.00 30.03	
٠.	ATOM	4071	CD.	GLU	201	20.954	19.773	54.457	1.00 32.95	В
	ATOM	4072	. OE1	GLU	201	20.075	19.784	55.345	1.00 34.01	В
15	ATOM	4073	OE2	GLU	201	20.817	19.167	53.367	1.00 33.38	В
	ATOM	4074	C	GLU	201	24.581	22.363	52.278	1.00 26.18	В
	ATOM	4075	ō	GLU	201	23.866	23.259	51.853	1.00 25.94	В
						25.707	21.996	51.674	1.00 25.78	В
	MOTA	4076	N	ILE	202					
20	MOTA	4077	CA	ILE	202	26.116	22.631	50.433	1.00 25.80	В
20	MOTA	4078	CB	ILE	202	27.636	22.813	50.360	1.00 25.61	. В
	ATOM	4079	CG2	ILE	202	28.022	23.102	48.914	1.00 25.19	В
	MOTA	4080		ILE	202	28.089	23.969	51.258	1.00 26.32	В
	ATOM	4081		ILE	202	27.704	23.871	52.722	1.00 25.98	В.
					202	25.655	21.820	49.231	1.00 26.76	·B
25	MOTA	4082	C	ILE						В
23	MOTA	4083	0	ILE	202	25.798	20.597	49.195	1.00 26.87	
	MOTA	4084	N	THR	203	25.089	22.508	48.248	1.00 26.89	В
	MOTA	4085	CA	THR	203	24.610	21.817	47.070	1.00 28.63	В
	ATOM	4086	CB	THR	203	. 23:463	22.606	46.329	1.00 28.93	В
	ATOM	4087	OG1	THR	203	22.297	22.683	47.167	1.00 28.96	В
30	ATOM	4088		THR	203	23.103	21.922	44.987	1.00 25.61	В
50						25.774	21.634	46.120	1.00 29.69	В
	MOTA	4089	С	THR	203					В
	ATOM	4090	0	THR	203	26.546	22.547	45.906	1.00 31.36	
	MOTA	4091	N	VAL	204	25.919	20.428	45.589	1.00 30.40	В
	MOTA	4092	CA	VAL	204	26.967	20.168	44.620	1.00 30.44	В
35	ATOM	.4093	CB	VAL	204	27.656	18.798	44.876	1.00 29.19	₿
	MOTA	4094		VAL	204	28.839	18.609	43.930	1.00 28.81	В
	ATOM	4095		VAL	204	28.142	18.733	46.292	1.00 29.07	В
						26.225	20.159	43.277	1.00 31.43	В
	MOTA	4096	Ç	VAL	204					В
40	MOTA	4097	٥	VAL	204	25.536	19.180	42.956	1.00 31.70	
40	MOTA	4098	N	HIS	205	26.354	21.255	42.521	1.00 31.11	В
	ATOM	4099	CA	HIS	205	25.709	21.420	41.214	1.00 30.37	В
	MOTA	4100	CB	HIS	205	25.803	22.869	40.792	1.00 29.29	В
	ATOM	4101	CG	HIS	205	25.131	23.788	41.747	1.00 29.35	В
	ATOM	4102		HIS	205	25.631	24.594	42.712	1.00 29.07	В
45						23.760	23.890	41.831	1.00 29.17	В
40	MOTA	4103		HIS	205					В
	MOTA	4104		HIS	205	23.444	24.721	42.806	1.00 29.14	
	MOTA	4105	NE2	HIS	205	24.561	25.161	43.357	1.00 29.64	В
	MOTA	4106	С	HIS	205	26.252	20.533	40.100	1.00 30.88	В
	MOTA	4107	0	HIS	205	25.508	20.130	39.216	1.00 31.82	В
50	ATOM	4108	N	ASN	206	27.544	20.238	40.138	1.00 29.74	В
. • •	ATOM	4109	CA	ASN	206	28.127	19.370	39.141	1.00 29.11	В
						28.377	20.158	37.852	1.00 28.48	В
	MOTA	4110	CB	ASN	206					В
	MOTA	4111	CG	ASN	206	29.156	21.438	38.091	1.00 29.29	
~ ~	MOTA	4112	OD1	ASN	206	30.252	21.412	38.645	1.00 28.71	В
55	ATOM	4113	ND2	ASN	206	28.594	22.562	37.673	1.00 28.54	В
	MOTA	4114	С	ASN	206	29.387	18.760	39.729	1.00 28.47	В
	MOTA	4115	0	ASN	206	29.740	19.032	40.852	1.00 27.98	В
	ATOM	4116	N	LYS	207	30.063	17.924	38.957	1.00 29.11	В
									1.00 30.00	В
40	MOTA	4117	CA	LYS	207	31.274	17.291	39.445		
60	MOTA	4118	CB	LYS	207	31.662	16.107	38.553	1.00 30.11	В
	MOTA	4119	CG	LYS	207	32.257	16.495	37.222	1.00 32.75	В
	MOTA	4120	CD	LYS	207	32.719	15.270	36.441	1.00 33.95	В
	MOTA	4121	CE	LYS	207	33.466	15.669	35.164	1.00 34.56	В
	MOTA	4122	NZ	LYS	207	34.775	16.370	35.404	1.00 33.30	B
65							18.293		1.00 30.73	В
U)	MOTA	4123	C	LYS	207	32.425		39.488		
	MOTA	4124	0	LYS	207	33.458	18.026	40.089	1.00 32.12	В
	MOTA	4125	N	ASP	208	32.241	19.451	38.863	1.00 29.02	В
	ATOM	4126	CA	ASP	208	33.301	20.453	38.850	1.00 28.26	В
	ATOM	4127	СВ	ASP	208	33.234	21.261	37.556	1.00 31.08	В
70	ATOM	4128	CG	ASP	208	33.702	20.463	36.354	1.00 32.65	В
, 0							20.729	35.233	1.00 33.84	В
	ATOM	4129		ASP	208	33.221				
	MOTA	4130		ASP	208	34.567	19.570	36.523	1.00 33.75	В
	MOTA	4131	С	ASP	208	33.277	21.374	40.065	1.00 26.42	В

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	MOTA	4132	0	ASP	208	33.989	22.372	40.117	1.00 24.98	В
	MOTA	4133	N	GLU	209	32.462	21.032	41.052 42.272	1.00 25.24 1.00 25.22	B B
	ATOM ATOM	4134 4135	CA CB	GLU	209 209	32.388 30.958	21.831 22.278	42.595	1.00 27.01	В
5	MOTA	4136	CG	GLU	209	30.306	23.237	41.602	1.00 30.48	В
_	MOTA	4137	CD	GLU	209	29.069	23.926	42.167	1.00 32.55	В
	MOTA	4138	OE1		209	28.371	24.610	41.385	1.00 34.80	В
	MOTA	4139	OE2	GLU	209	28.804	23.793	43.382	1.00 33.17	В
10	ATOM	4140	C	GLU	209	32.832	21.030	43.490	1.00 24.23 1.00 25.15	B
10	MOTA MOTA	4141 4142	N	GLU VAL	209 210	33.194 32.835	21.596 19.708	44.513	1.00 21.99	В
	MOTA	4143	CA	VAL	210	33.205	18.882	44.514	1.00 18.98	В
	MOTA	4144	СВ	VAL	210	32.987	17.360	44.217	1.00 17.62	В
	MOTA	4145	CG1	VAL	210	32.238	17.180	42.928	1.00 17.92	В
15	MOTA	4146	CG2		210	34.290	16.638	44.159	1.00 17.49	В
	MOTA	4147	C	VAL	210	34.609	19.093 19.138	45.082 46.289	1.00 18.13 1.00 19.29	B
	MOTA MOTA	4148 4149	. O	VAL TYR	210 211	34.775 35.620	19.138	44.232	1.00 17.72	В
	ATOM	4150	CA	TYR	211	36.968	19.401	44.770	1.00 15.84	В
20	MOTA	4151	СВ	TYR	211	38.030	19.361	43.656	1.00 14.23	В
	MOTA	4152	CG	TYR	211	39.441	19.224	44.196	1.00 13.57	В
	MOTA	4153	CD1	TYR	211	39.807	18.110	44.937	1.00 12.81	B B
	MOTA	4154 4155	CE1	TYR TYR	211 211	41.062 40.379	18.018 20.246	45.528 44.048	1.00 12.54 1.00 14.65	В
25	ATOM ATOM	4156		TYR	211	41.651	20.166	44.642	1.00 13.74	В
	ATOM	4157	cz	TYR	211	41.987	19.048	45.386	1.00 14.45	В
	MOTA	4158	OH	TYR	211	43.235	18.972	45.997	1.00 10.15	В
	MOTA	4159	С	TYR	211	37.083	20.665	45.608	1.00 15.70	В
30	MOTA	4160	0	TYR	211	37.626 36.557	20.620 21.781	46.696 45.101	1.00 14.92 1.00 17.75	B B
20	MOTA MOTA	4161 4162	N CA	GLN	212 212	36.582	23.064	45.819	1.00 18.64	В
	ATOM	4163	СВ	GLN	212	35.897	24.154	44.983	1.00 19.40	В
	ATOM	4164	CG	GLN	212	35.962	25.543	45.607	1.00 24.51	В
25	MOTA	4165	CD	GLN	212	35.764	26.672	44.587	1.00 26.82	В
35	MOTA	4166		GLN	212	35.046	26.508	43.594 44.844	1.00 25.33 1.00 26.86	B B
	MOTA MOTA	4167 4168	NE2	GLN	212 212	36.391 35.909	27.832 22.923	47.192	1.00 18.53	В
	ATOM	4169	ō	GLN	212	36.420	23.374	48.193	1.00 19.69	В
	ATOM	4170	N	ILE	213	34.759	22.265	47.230	1.00 19.83	B
40	MOTA	4171	CA	ILE	213	34.031	22.048	48.485	1.00 19.97	В
	ATOM	4172	CB	ILE	213	32.664	21.350	48.237	1.00 20.59	B B
	MOTA	4173 4174		ILE	213 213	32.022 31.758	20.933	49.579 47.441	1.00 19.77 1.00 20.66	В
	MOTA MOTA	4175		ILE	213	30.505	21.626	46.928	1.00 22.87	В
45	MOTA	4176	c	ILE	213	34.831	21.189	49.461	1.00 20.10	В
	MOTA	4177	0	ILE	213	34.822	21.446	50.672	1.00 20.46	В
	MOTA	4178	N	LEU	214	35.489	20.156	48.937	1.00 19.00	В
	MOTA	4179 4180	CA CB	LEU	214 214	36.310 36.829	19.282 18.100	49.759 48.950	1.00 18.96 1.00 18.27	B B
50	MOTA MOTA	4181	CG	LEU	214	36.013	16.826	49.015	1.00 18.28	В
	ATOM	4182		LEU	214	34.547	17.179	48.926	1.00 22.38	В
	MOTA	4183		LEU	214	36.443	15.908	47.895	1.00 17.95	В
	MOTA	4184	С	LEU	214	37.507	20.048	50.316	1.00 19.17	В
55	MOTA	4185	0	LEU	214	37.920	19.821 20.967	51.443 49.523	1.00 20.21 1.00 19.88	B B
23	MOTA	4186 4187	N CA	GLU	215 215	38.055 39.208	21.768	49.953	1.00 19.18	В
	ATOM	4188	СВ	GLU	215	39.748	22.628	48.797	1.00 19.26	В
	ATOM	4189	CG	GLU	215	40.496	21.863	47.699	1.00 20.08	В
	ATOM.	4190	CD	GLU	215	41.103	22.786	46.630	1.00 20.78	В
60	ATOM	4191		GLU	215	42.352	22.898	46.580	1.00 16.87	В
	MOTA	4192		GLU	215	40.337	23.399	45.842 51.110	1.00 19.38 1.00 18.78	B B
	MOTA MOTA	4193 4194	0	GLU	215 215	38.855 39.592	22.700 22.798	52.092	1.00 17.36	В
	ATOM	4195	N	LYS	216	37.732	23.397	50.988	1.00 19.53	В
65	ATOM	4196	CA	LYS	216	37.293	24.300	52.042	1.00 20.63	В
	MOTA	4197	CB	LYS-	216	35.993	24.988	51.620	1.00 22.77	В
	ATOM	4198	CG	LYS	216	36.240	26.094	50.602	1.00 29.39	В
	MOTA	4199	CD	LYS	216	34.962	26.743	50.069 49.187	1.00 33.26 1.00 35.91	B B
70	MOTA MOTA	4200 4201	CE NZ	LYS	216 216	35.281 36.198	27.963 27.671	48.028	1.00 35.91	В
, ,	ATOM	4202	C	LYS	216	37.144	23.547	53.361	1.00 20.03	В
	MOTA	4203	ō	LYS	216	37.501	24.057	54.416	1.00 21.40	В
	MOTA	4204	N	GLY	217	36.628	22.329	53.309	1.00 18.86	В

	MOTA	4205	CA	GLY	217	36.492	21.587	54.543	1.00 18.29	В
	MOTA	4206	С	GLY	217	37.869	21.334	55.128	1.00 18.39	В
	MOTA	4207	D	GLY	217	38.103	21.531	56.307	1.00 18.74	В
	MOTA	4208	N	ALA	218	38.792	20.895	54.282	1.00 19.27	В
5	MOTA	4209	CA	ALA	218	40.148	20.607	54.737	1.00 19.03	В
	MOTA	4210	CB	ALA	218	40.996	20.061	53.580	1.00 18.52	В
	MOTA	4211	C	ALA	218	40.827	21.818	55.363	1.00 18.17	В
	MOTA	4212	0	ALA	218	41.470	21.706	56.403	1.00 19.12	В
• •	MOTA	4213	N	ALA	219	40.691	22.980	54.735	1.00 17.99	. В
10	MOTA	4214	CA	ALA	219	41.315	24.203	55.266	1.00 16.17	B
	MOTA	4215	·CB	ALA	219	41.044	25.404	54.323	1.00 14.07	В
	MOTA	4216	С	ALA	219	40.792	24.505	56.671	1.00 14.78	В
	MOTA	4217	0	ALA	219	41.552	24.760	57.599	1.00 15.56	В
1.5	MOTA	4218	N	LYS	220	39.479	24.450	56.823	1.00 14.00	В
15	MOTA	4219	CA	LYS	220	38.859	24.729	58.110	1.00 13.80	В
	ATOM	4220	CB	LYS	220	37.338	24.667	57.978	1.00 11.84	В
	MOTA	4221	CG	LYS	220	36.603	25.222	59.177	1.00 12.63	В
	MOTA	4222	CD	LYS	220	35.130	25.462	58.884	1.00 11.67	B B
20	MOTA	4223	CE	LYS	220	34.464	26.087	60.092	1.00 13.88	. В
20	MOTA	4224	NS	LYS	220	32.993	26.287	59.939	1.00 12.51 1.00 14.26	. В
	MOTA	4225	c	LYS	220	39.303	23.734	59.173 60.350	1.00 15.25	В
	MOTA	4226	0	LYS	220	39.442	24.067	58.748	1.00 14.19	В.
	MOTA	4227	N	ARG	221	39.513 39.936	22.498 21.438	59.647	1.00 11.64	·B
25	MOTA	4228	CA	ARG	221	39.878	20.111	58.889	1.00 13.12	В
23	MOTA	4229	CB	ARG	221 221	40.038	18.857	59.751	1.00 13.06	В
	ATOM ATOM	4230 4231	CD	ARG	221	39.999	17.586	58.902	1.00 11.48	В
	MOTA	4232	NE	ARG	221	38.638	17.093	58.691	1.00 8.87	В
	ATOM	4233	CZ	ARG	221	38.317	16.184	57.774	1.00 8.38	В
30	ATOM	4234		ARG	221	39.255	15.687	56.976	1.00 5.16	В
20	ATOM	4235		ARG	221	37.074	15.732	57.687	1.00 8.15	В
	MOTA	4236	C	ARG	221	41.345	21.737	60.174	1.00 10.67	В
	MOTA	4237	ō	ARG	221	41.686	21.394	61.314	1.00 10.15	В
	MOTA	4238	N	THR	222	42.167	22.372	59.342	1.00 10.52	В
35	ATOM	. 4239	CA	THR	222	43.515	22.747	59.752	1.00 7.37	В
	ATOM	4240	CB	THR	222	44.277	23.438	58.634	1.00 6.75	В
	ATOM	4241	OG1		222	44.586	22.466	57.637	1.00 9.09	В
	MOTA	4242	CG2		222	45.573	24.026	59.136	1.00 5.92	В
	ATOM	4243	C	THR	222	43.475	23.692	60.916	1.00 5.52	В
40	ATOM	4244	o	THR	222	44.265	23.598	61.797	1.00 6.41	В
	MOTA	4245	N	THR	223	42.527	24.607	60.906	1.00 5.73	В
	ATOM	4246	CA	THR	223	42.443	25.550	61.990	1.00 7.41	В
	ATOM	4247	CB	THR	223	41.481	26.706	61.654	1.00 9.80	В
	MOTA	4248	OG1	THR	223	40.126	26.260	61.807	1.00 13.96	В
45	MOTA	4249	CG2	THR	223	41.716	27.205	60.212	1.00 11.03	В
	MOTA	4250	С	THR	223	41.941	24.801	63.206	1.00 8.79	В
	MOTA	4251	0	THR	223	42.353	25.101	64.337	1.00 11.00	В
	MOTA	4252	N	ALA	224	41.093	23.796	62.970	1.00 9.46	В
~^	MOTA	4253	CA	ALA	224	40.537	23.001	64.069	1.00 9.41	В
50	MOTA	4254	CB	ALA	224	39.514	21.966	63.570	1.00 8.72	В
	ATOM	4255	С	ALA	224	41.645	22.288	64.798	1.00 10.87	В
	MOTA	4256	0	ALA	224	41.693	22.258	66.041	1.00 10.92	В
	MOTA	4257	N	ALA	225	42.526	21.678	64.020	1.00 11.03	В
<i></i>	MOTA	4258	CA	ALA	225	43.647	20.977	64.608	1.00 10.24	В
55	MOTA	4259	CB	ALA	225	44.484	20.347	63.517	1.00 9.24	В
	MOTA	4260	С	ALA	225	44.502	21.942	65.446	1.00 11.63	В
	MOTA	4261	0	ALA	225	44.983	21.592	66.516	1.00 12.58	В
	MOTA	4262	N	THR	226	44.676	23.164	64.957	1.00 13.45	В.
40	ATOM	4263	CA	THR	226	45.490	24.156	65.650	1.00 15.18	В
60	ATOM	4264	CB	THR	226	45.557	25.470	64.868	1.00 14.69	В
	MOTA	4265		THR	226	46.323	25.286	63.670	1.00 16.29	В
	MOTA	4266		THR	226	46.186	26.534	65.716	1.00 15.17	В
	MOTA	4267	С	THR	226	44.901	24.452	67.007	1.00 16.64	В
65	ATOM	4268	0	THR	226	45.617	24.553	67.998	1.00 18.41	B B
O)	HOTA	4269	N	LEU	227	43.575	24.575	67.025	1.00 18.18	В
	ATOM	4270	CA	LEU	227	42.805	24.875	68.238 67.899	1.00 18.74	В
	MOTA	4271	CB	LEU	227	41.367	25.310	68.051	1.00 19.87	В
	MOTA	4272	CG	LEU	227	40.955	26.772 27.134	69.518	1.00 21.88	В
70	MOTA	4273		LEU	227	41.103	27.134	67.155	1.00 21.51	В
70	MOTA	4274		LEU	227	41.786	27.693	69.239	1.00 21.31	В
	MOTA	4275	C	LEU	227	42.651 42.783	23.733	70.435	1.00 18.61	В
	MOTA	4276	Ο.	LEU	227	42.783	22.536	68.742	1.00 18.27	В
	MOTA	4277	N	MET	228	74.700		JJ. 172		_

	MOTA	4278	CA	MET	228	42.160	21.404	69.634	1.00 1	7 51	В
	MOTA	4279	CB	MET	228	40.800	20.772	69.302	1.00 1		В
	MOTA	4280	CG	MET	228	39.649	21.745	69.495	1.00 1		В
	MOTA	4281	SD	MET	228	38.056	21.201	68.874	1.00 1	9.18	В
5	MOTA	4282	CE	MET	228	38.092	22.153	67.250	1.00 1	7.21	В
_				MET	228	43.250	20.342	69.614	1.00 1		В
	ATOM .	4283	C								
	MOTA	4284	0	MET	228	43.769	19.990	68.549	1.00 2		. В
	MOTA	4285	N	ASN	229	43.571	19.834	70.807	1.00 1	6.66	В
	ATOM	4286	CA	ASN	229	44.589	18.799	70.992	1.00 1	6.35	В
10					229			72.485	1.00 1		В
10	MOTA	4287	CB	ASN		44.824	18.543				
	MOTA	4288	CG	ASN	229	45.350	19.764	73.209	1.00 1		В
	ATOM	4289	OD1	ASN	229	45.764	20.739	72.588	1.00 1	7.78	В
	ATOM	4290	ND2	ASN	229	45.340	19.711	74.534	1.00 1	4.68	В
	ATOM	4291	С	ASN	229	44.311	17.448	70.313	1.00 1		В
15											В
IJ	MOTA	4292	0	ASN	229	43.228	16.873	70.460	1.00 1		
	ATOM	4293	N	ALA	230	45.300	16.950	69.569	1.00 1		₽
	MOTA	4294	CA	ALA	230	45.171	15.679	68.863	1.00 1	2.00	В
	MOTA	4295	СВ	AŁA	230	45.241	14.546	69.847	1.00 1	1.64	В
				ALA	230	43.869	15.595	68.079	1.00 1		В
20 .	MOTA	4296	С								
20	MOTA	4297	0	ALA	230	43.269	14.519	67.977	1.00 1		В
	MOTA	4298	N	TYR	231	43.443	16.725	67.519	1.00 1	.1.27	В
	ATOM	4299	CA	TYR	231	42.200	16.775	66.761	1.00 1	2.69	В.
	ATOM	4300	CB	TYR	231	42.047	18.119	66.029	1.00 1	1.10	В
								65.435	1.00 1		·B
25	MOTA	4301	CG	TYR	231	40.667	18.312				
25	MOTA	4302	CD1	TYR	231	40.404	17.998	64.112	1.00	9.88	В
	MOTA	4303	CE1	TYR	231	39.121	18.122	63.598	1.00 1	0.11	В
	MOTA	4304	CD2	TYR	231	39.606	18.760	66.229	1.00 1	1.37	В
	MOTA	4305	CE2	TYR	231	38.316	18.886	65.716	1.00 1	0.13	В
				TYR		38.079	18.559	64.402	1.00	9.90	В
20	MOTA	4306	CZ		231						
30	MOTA	4307	ОН	TYR	231	36.780	18.623	63.936	1.00	7.41	В
	MOTA	4308	С	TYR	231	41.988	15.645	65.748	1.00 1	.3.47	В
	MOTA	4309	0	TYR	231	41.016	14.916	65.837	1.00 1	4.47	В
	ATOM	4310	N	SER	232	42.904	15.481	64.800	1.00 1		В
	MOTA				232	42.744	14.446	63.777	1.00		B
35 [·]		4311	CA	SER							
33	MOTA	4312	CB	SER	232	43.907	14.490	62.779	1.00		В
	MOTA	4313	OG	SER	232	45.145	14.290	63.419	1.00 2	20.92	В
	MOTA	4314	С	SER	232	42.608	13.020	64.308	1.00 1	5.28	В
	ATOM	4315	0	SER	232	41.898	12.203	63.726	1.00 1	6.22	В
		4316			233	43.260	12.711	65.417	1.00 1		В
40	MOTA		N	SER							
40	ATOM	4317	CA	SER	233	43.173	11.352	65.919	1.00 1		В
	MOTA	4318	CB	SER	233	44.477	10.942	66.596	1.00 1	13.54	В
	MOTA	4319	OG	SER	233	44.662	11.602	67838	1.00 1	15.82	В
	MOTA	4320	С	SER	233	42.057	11.167	66.921	1.00 1	2.47	В
	MOTA	4321	ŏ	SER	233	41.604	10.047	67.155	1.00		В
45											
43	MOTA	4322	N	ARG	234	41.612	12.265	67.523	1.00 1		В
	MOTA	4323	CA	ARG	234	40.558	12.168	68.532	1.00	9.69	В
	MOTA	4324	CB	ARG	234	40.919	12.961	69.784	1.00 1	10.96	В
	MOTA	4325	CG	ARG	234	41.315	12.112	70.975	1.00 1	13.22	В
	ATOM	4326	CD	ARG	234	42.707	12.435	71.494	1.00 1		В
50											В
50	MOTA	4327	NE	ARG	234	42.755	13.676	72.263	1.00 2		
	MOTA	4328	CZ	ARG	234	43.751	14.005	73.083	1.00 2		В
	ATOM	4329	NH1	ARG	234	44.791	13.186	73.242	1.00 2	22.37	B
	MOTA	4330	NH2	ARG	234	43.690	15.140	73.767	1.00	25.64	В
	ATOM	4331	C .	ARG	234	39.168	12.617	68.118	1.00	7.73	В
55		4332	ŏ.	ARG	234	38.258	12.599	68.924	1.00	8.22	В
22	MOTA		•								
	ATOM	4333	N	SER	235	39.006	13.014	66.862	1.00	6.52	В
	ATOM	4334	CA	SER	235	37.697	13.455	66.394	1.00	4.31	В
	MOTA	4335	CB	SER	235	37.785	14.801	65.647	1.00	2.24	В.
	ATOM	4336	OG.	SER	235	38.745	14.780	64.602	1.00	1.00	В
60			c	SER	235	37.048	12.437	65.488	1.00	2.58	В
oo	MOTA	4337									
	MOTA	4338	0	SER	235 ·	37.704	11.648	64.854	1.00	3.58	В
	ATOM	4339	N	HIS	236	35.725	12.465	65.472	1.00	4.87	В
	ATOM	4340	CA	HIS	236	34.911	11.587	64.631	1.00	5.05	В
	MOTA	4341	CB	HIS	236	33.691	11.087	65.386	1.00	4.65	В
65											
J	MOTA	4342	CG	HIS	236	34.032	10.280	66.586	1.00	4.01	В
	MOTA	4343		HIS	236	34.066	10.607	67.899	1.00	3.63	В
	ATOM	4344	ND1	HIS	236	34.437	8.965	66.504	1.00	3.84	В
	MOTA	4345		HIS	236	34.704	8.517	67.717	1.00	4.48	В
	MOTA	4346		HIS	236	34.487	9.494	68.582	1.00	4.72	В
70											
, 0	MOTA	4347	C	HIS	236	34.347	12.498	63.556	1.00	6.99	. В
	MOTA	4348	0	HIS	236	33.810	13.556	63.878	1.00	9.70	В
	ATOM	4349	N	SER	237	34.475	12.108	62.291	1.00	7.23	В
	MOTA	4350	CA	SER	237	33.951	12.933	61.208	1.00	6.69	В
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	MOTA	4351	CB	SER	237	35.058	13.406	60.253	1.00 5.37	В
	ATOM	4352	OG	SER	237	35.464	12.358	59.380	1.00 3.60	В
	MOTA	4353	C	SER	237	32.946	12.157	60.393	1.00 7.89 1.00 9.95	B
5	MOTA MOTA	4354 4355	N N	SER VAL	237 238	33.196 31.787	11.040 12.753	59.976 60.180	1.00 7.91	В
,	MOTA	4356	CA	VAL	238	30.787	12.078	59.392	1.00 7.74	В
	ATOM	4357	СВ	VAL	238	29.560	11.740	60.282	1.00 8.04	В
	ATOM	4358		VAL	238	29.413	12.787	61.328	1.00 7.80	В
	ATOM	4359	CG2	VAL	238	28.307	11.669	59.460	1.00 8.71	В
10	MOTA	4360	С	VAL	238	30.421	12.935	58.182	1.00 8.25	В
	MOTA	4361	0	VAL	238	29.776	13.952	58.323	1.00 9.09	В
	MOTA	4362	N	PHE	239	30.883	12.511	57.002	1.00 8.31	В
	MOTA	4363	CA	PHE	239	30.609	13.198	55.732 54.759	1.00 8.81 1.00 6.73	B B
15	MOTA MOTA	4364 4365	CB	PHE	239 239	31.793 31.693	13.036 13.893	53.525	1.00 6.12	В
13	MOTA	4366		PHE	239	30.815	13.557	52.500	1.00 5.69	В
	ATOM	4367		PHE	239	32.462	15.046	53.394	1.00 5.95	· B
	ATOM	4368		PHE	239	30.705	14.364	51.348	1.00 5.30	В
00	MOTA	4369	CE2	PHE	239	32.354	15.854	52.247	1.00 5.11	B
20	MOTA	4370	CZ	PHE	239	31.475	15.511	51.224	1.00 3.58	В
	MOTA	4371	С	PHE	239	29.350	12.553	55.148	1.00 9.90	В
	MOTA	4372	0	PHE	239	29.327	11.356	54.859	1.00 9.81 1.00 10.63	B B
	MOTA MOTA	4373 4374	N CA	SER	240 240	28.305 27.039	13.359 12.871	54.982 54.466	1.00 10.03	В
25	MOTA	4375	CB	SER	240	25.926	13.194	55.467	1.00 9.24	В
	MOTA	4376	OG	SER	240	26.182	12.631	56.742	1.00 8.98	. в
	MOTA	4377	c	SER	240	26.678	13.462	53.105	1.00 10.23	В
	MOTA	4378	0	SER	240	26.809	14.668	52.877	1.00 10.82	В
20	MOTA	4379	N	VAL	241	26.230	12.601	52.198	1.00 10.77	В
30	ATOM	4380	CA	VAL	241	25.813	13.044	50.874	1.00 12.14	В
	ATOM	4381 4382	CB	VAL	241 241	26.748 26.981	12.492 11.008	49.775 50.002	1.00 12.12 1.00 13.27	B B
	MOTA MOTA	4382 4383		VAL	241	26.143	12.736	48.394	1.00 11.17	В
	MOTA	4384	C	VAL	241	24.379	12.565	50.649	1.00 13.61	В
35	ATOM	4385	ō	VAL	241	24.092	11.365	50.700	1.00 13.01	В
	MOTA	4386	N	THR	242	23.478	13.513	50.422	1.00 14.36	В
	ATOM	4387	CA	THR	242	22.078	13.203	50.217	1.00 16.18	В
	ATOM	4388	CB	THR	242	21.198	14.104	51.118	1.00 17.52	В
40	ATOM	4389		THR	242	21.546	13.897	52.496 50.954	1.00 19.73	B B
40	MOTA MOTA	4390 4391	CG2 C	THR	242 242	19.738 21.746	13.766 13.418	48.741	1.00 20.45	В
	ATOM	4392	ō	THR	242	22.212	14.357	48.128	1.00 19.20	В
	ATOM	4393	N	ILE	243	20.945	12.521	48.180	1.00 20.44	В
4.5	MOTA	4394	CA	ILE	243	20.560	12.619	46.785	1.00 23.13	В
45	MOTA	4395	CB	ILE	243	21.178	11.477	45.941	1.00 22.27	В
	ATOM	4396		ILE	243	20.962	11.770	44.475	1.00 18.06	В
	ATOM	4397		ILE	243	22.663	11.310	46.270 45.722	1.00 21.29	B B
	MOTA MOTA	4398 4399	CDI	ILE	243 243	23.247 19.043	10.072 12.555	46.628	1.00 26.42	В
50	ATOM	4400	ō	ILE	243	18.442	11.488	46.790	1.00 27.92	В
	ATOM	4401	N	HIS	244	18.437	13.707	46.340	1.00 29.29	В
	MOTA	4402	CA	HIS	244	17.001	13.808	46.117	1.00 30.50	В
	MOTA	4403	CB	HIS	244	16.486	15.226	46.393	1.00 31.87	В
55 .	ATOM	4404	CG	HIS	244	16.375	15.565	47.845	1.00 34.67	В
55	MOTA	4405		HIS	244	15.341	15.441	48.712	1.00 35.28	B B
	ATOM	4406 4407		HIS	244 244	17.424 17.040	16.087 16.267	48.577 49.828	1.00 36.67	В
	MOTA MOTA	4408		HIS	244	15.778	15.881	49.936	1.00 35.59	В
	ATOM	4409	C	HIS	244	16.803	13.494	44.637	1.00 32.12	В
60	ATOM	4410	ō	HIS	244	17.277	14.228	43.755	1.00 32.44	В
	MOTA	4411	N	MET	245	16.122	12.388	44.368	1.00 32.37	В
	ATOM	4412	CA	MET	245	15.877	11.968	42.998	1.00 32.37	В
	MOTA	4413	СB	MET	245	16.475	10.578	42.791	1.00 31.86	В
65	MOTA	4414	CG	MET	245	17.968	10.548	43.055	1.00 31.73	В
65	MOTA	4415	SD	MET	245	18.589	8.875	43.225	1.00 33.02	В
-	MOTA MOTA	4416 4417	CE	MET	245 245	18.034 14.401	8.477 12.002	44.892 42.601	1.00 31.10	B B
	ATOM	4417	0	MET	245	13.509	11.738	43.415	1.00 31.83	В
	ATOM	4419	N	LYS	246	14.159	12.334	41.337	1.00 31.84	8
70	MOTA	4420	CA	LYS	246	12.811	12.428	40.804	1.00 31.99	В
	MOTA	4421	CB	LYS	246	12.350	13.895	40.781	1.00 32.10	В
	MOTA	4422	CG	LYS	246	10.922	14.087	40.292	1.00 34.26	В
	MOTA	4423	CD	LYS	246	10.606	15.539	39.946	1.00 34.52	В

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	MOTA	4424	CE	LYS	246	10.646	16:433	41.173	1.00 36.15	В
	MOTA	4425	NZ	LYS	246	10.457	17.872	40.836	1.00 35.42	В
	ATOM	4426	c	LYS	246	12.761	11.870	39.382	1.00 31.58	В
	MOTA	4427	ō	LYS	246	13.439	12.358	38.480	1.00 30.24	В
5									1.00 31.71	В
,	MOTA	4428	N	GLU	247	11.967	10.824	39.196		
	MOTA	4429	CA	GLU	247	11.808	10.238	37.874	1.00 30.99	В
	MOTA	4430	СВ	GLU	247	12.337	8.801	37.855	1.00 32.21	В
	MOTA	4431	CG	GLU	247	11.815	7.897	38.961	1.00 33.61	В
	ATOM	4432	CD	GLU	247	12.672	6.647	39.115	1.00 35.27	В
10	ATOM	4433		GLU	247	12.420	5.841	40.037	1.00 35.63	B
	MOTA	4434	OE2		247	13.609	6.469	38.307	1.00 35.39	В
							10.298	37.479	1.00 30.04	В
	ATOM	4435	C	GLU	247	10.338				
	MOTA	4436	0	GLU	247	9.448	10.169	38.317	1.00 29.68	В
	MOTA	4437	N	THR	248	10.083	10.513	36.197	1.00 28.13	В
15	MOTA	4438	CA	THR	248	8.716	10.591	35.720	1.00 26.83	В
	MOTA	4439	CB	THR	248	8.506	11.895	34.942	1.00 25.80	В
•	MOTA	4440		THR	248	8.937	12.995	35.750	1.00 24.67	В
	ATOM	4441		THR	248	7.046	12.096	34.617	1.00 25.62	В
	ATOM	4442	c	THR	248	8.406	9.395	34.822	1.00 26.77	В
20						9.168	9.077	33.914	1.00 27.38	В
20	MOTA	4443	0	THR	248					
	MOTA	4444	N	THR	249	7.288	8.732	35.092	1.00 26.76	В
	MOTA	4445	CA	THR	249	6.877	7.580	34.302	1.00 26.72	В.
	MOTA	4446	CB	THR	249	5.759	6.784	35.011	1.00 26.45	В
	MOTA	4447	0G1	THR	249	4.575	7.587	35.088	1.00 27.92	· B
25	ATOM	4448		THR	249	6.180	6.404	36.423	1.00 25.26	В
	ATOM	4449	c	THR	249	6.353	8.040	32.938	1.00 27.55	В
		4450			249	6.316	9.226	32.638	1.00 27.26	В
	MOTA		0	THR					1.00 29.51	В
	MOTA	4451	N	ILE	250	5.956	7.078	32.113		
20	MOTA	4452	CA	ILE	250	5.434	7.353	30.774	1.00 30.16	В
30	MOTA	4453	CB	ILE	250	5.444	6.074	29.901	1.00 29.03	В
	MOTA	4454	CG2	ILE	250	4.410	5.082	30.421	1.00 27.86	В
	ATOM	4455	CG1	ILE	250	5.157	6.431	28.443	1.00 28.33	В
	MOTA	4456		ILE	250	5.425	5.295	27.476	1.00 26.91	В
	ATOM	4457	c	ILE	250	4.005	7.884	30.877	1.00 31.97	В
.35					250	3.400	8.286	29.891	1.00 31.50	В
.55	MOTA	4458	0	ILE						В
	MOTA	4459	N	ASP	251	3.477	7.875	32.095	1.00 34.02	
	MOTA	4460	CA	ASP	251	2.132	8.368	32.359	1.00 36.26	В
	MOTA	4461	CB	ASP	251	1.425	7.469	33.381	1.00 36.12	В
	MOTA	4462	CG	ASP	251	0.789	6.242	32.750	1.00 36.40	В
40	MOTA	4463	OD1	ASP	251	0.223	5.420	33.509	1.00 34.19	В
	MOTA	4464		ASP	251	0.854	6.119	31.504	1.00 36.03	В
	ATOM	4465	c	ASP	251	2.164	9.804	32.910	1.00 37.47	В
	ATOM	4466	ō	ASP	251	1.140	10.468	32.990	1.00 38.11	В
										В
45	MOTA	4467	N	GLY	252	3.350	10.273	33.284	1.00 37.77	
43	MOTA	4468	CA	GLY	252	3.471	11.613	33.822	1.00 37.41	В
	MOTA	4469	С	GLY	252	3.566	11.662	35.338	1.00 38.71	В
	ATOM	4470	0	GLY	252	3.747	12.734	35.912	1.00 38.78	В
	MOTA	4471	N	GLU	253	3.440	10.516	36.003	1.00 38.85	В
	MOTA	4472	CA:	GLU	253	3.533	10.511	37.459	1.00 39.67	В
50	ATOM	4473	СВ	GLU	253	3.020	9.200	38.052	1.00 41.37	В
-	ATOM	4474	CG	GLU	253	3.181	9.143	39.573	1.00 43.75	В
	ATOM					2.814	7.803	40.188	1.00 44.31	В
		4475	CD	GLU	253 .				1.00 44.42	В
	MOTA	4476		GLU	253	3.083	7.612	41.398		
~ ~	MOTA	4477	0E2	GLU	253	2.256	6.945	39.470	1.00 45.10	В
55	MOTA	4478	С	GLU	253	4.988	10.668	37.883	1.00 39.49	В
	MOTA	4479	0	GLU	253	5.890	10.286	37.149	1.00 39.20	B
	ATOM	4480	N	GLU	254	5.210	11.239	39.064	1.00 39.27	В
	ATOM	4481	CA	GLU	254	6.568	11.426	39.567	1.00 40.50	В.
		4482		GLU	254	6.793	12.875	39.978	1.00 41.13	В
60	ATOM		CB							В
UU	MOTA	4483	CG	GLU	254	6.621	13.842	38.836	1.00 44.09	
	ATOM	4484		GLU	254	7.073	15.233	39.189	1.00 45.25	В
	MOTA	4485	OE1	GLU	254	6.665	15.737	40.256	1.00 45.35	В
	MOTA	4486	OE2	GLU	254	7.828	15.825	38.391	1.00 46.38	В
	ATOM.	4487	C	GLU	254	6.926	10.539	40.756	1.00 39.50	В
65	ATOM	4488	ō	GLU	254	6.242	10.540	41.769	1.00 40.75	В
	ATOM	4489				8.008	9.779	40.614	1.00 37.82	В
			N	LEU	255					
	MOTA	4490	CA	LEU	255	8.484	8.894	41.676	1.00 36.11	В
	ATOM	4491	CB	LEU	255	8.895	7.543	41.087	1.00 35.93	В
70	MOTA	4492	CG	LEU	255	7.950	6.910	40.062	1.00 35.67	. В
70	ATOM	4493	CD1	LEU	255	8.538	5.614	39.590	1.00 35.24	В
	ATOM	4494		LEU	255	6.601	6.663	40.668	1.00 35.26	В
	MOTA	4495	C.	LEU	255	9.710	9.551	42.322	1.00 35.19	В
	ATOM	4496	o .	LEU	255	10.722	9.754	41.644	1.00 35.09	В
		- 470	_			10.,22	2.,21		1.00 33.07	_

	MOTA	4497	N	VAL	256	9.612	9.888	43.615	1.00 33.29	В
	ATOM	4498	CA	VAL	256	10.719	10.528	44.350	1.00 31.53	В
	MOTA	4499	CB	VAL	256	10.237	11.748	45.143	1.00 31.44	В
	ATOM	4500		VAL	256	9.719	12.800	44.188	1.00 30.73	В
5	ATOM	4501	CG2	VAL	256	9.165	11.322	46.141	1.00 33.02	В
,	ATOM	4502	c	VAL	256	11.494	9.622	45.319	1.00 29.50	В
		4503	ō	VAL	256	10.928	8.958	46.189	1.00 29.05	В
	ATOM ·	4504					9.604	45.148	1.00 27.07	В
	ATOM		N	LYS	257	12.809			1.00 24.38	В
10	ATOM ·	4505	CA	LYS	257	13.676	8.790	45.985		
10	MOTA	4506	CB	LYS	257	14.530	7.832	45.134	1.00 21.73	В
	MOTA	4507	CG	LYS	257	13.742	6.776	44.369	1.00 18.70	В
	MOTA	4508	CD	LYS	257	14.637	5.862	43.566	1.00 13.96	В
	MOTA	4509	CE	LYS	257	15.316	6.632	42.460	1.00 12.43	В
• -	MOTA	4510	NZ	LYS	257	16.093	5.743	41.576	1.00 10.28	В
15	ATOM	4511	С	LYS	257	14.627	9.701	46.731	1.00 23.77	В
	MOTA	4512	0	LYS	257	15.062	10.708	46.215	1.00 24.31	В
	ATOM	4513	N	ILE	258	14.928	9.357	47.970	1.00 22.97	В
	MOTA	4514	CA	ILE	258	15.882	10.138	48.741	1.00 20.65	₿
	ATOM	4515	CB	ILE	258	15.226	10.866	49.913	1.00 22.22	В
20	ATOM	4516	CG2	ILE	258	16.246	11.747	50.591	1.00 22.81	В
	ATOM	4517	CG1	ILE	258	14.080	11.734	49.407	1.00 24.53	Ð
	ATOM	4518	CD1	ILE	258	13.276	12.417	50.518	1.00 24.98	В
	ATOM	4519	С	ILE	258	16.891	9.136	49.271	1.00 18.47	В
	ATOM	4520	0	ILE	258	16.554	8.243	50.049	1.00 16.24	В
25	MOTA	4521	N	GLY	259	18.123	9.256	48.805	1.00 17.79	В
	MOTA	4522	CA	GLY	259	19.144	8.342	49.262	1.00 18.70	В
	ATOM	4523	c	GLY	. 259	20.205	9.094	50.030	1.00 17.80	В
	MOTA	4524	õ	GLY	259	20.684	10.110	49.555	1.00 18.70	В
	MOTA	4525	N	LYS	260	20.565	8.606	51.215	1.00 16.12	В
30	ATOM	4526	CA	LYS	260	21.598	9.263	52.011	1.00 15.58	В
50	ATOM	4527	CB	LYS	260	21.034	9.800	53.335	1.00 15.55	В
	ATOM	4528	CG	LYS	260	21.889	10.844	54.046	1.00 14.21	В
	MOTA	4529	CD	LYS	260	21.173	11.288	55.341	1.00 15.40	В
	ATOM	4530	CE		260		12.289	56.170	1.00 13.76	В
35				LYS		21.989		57.451	1.00 8.49	В
55	MOTA	4531	NZ	LYS	260	21.311	12.687			В
	MOTA	4532	C	LYS	260	22.729	8.309	52.335	1.00 13.87 1.00 13.84	В
	ATOM	4533	0	LYS	260	22.531	7.185	52.741	1.00 13.04	В
	MOTA	4534	N	LEU	261	23.937	8.788	52.141		
40	MOTA	4535	CA	LEU	261	25.107	7.996	52.430	1.00 11.82	В
40	MOTA	4536	CB	LEU	261	25.890	7.772	51.130	1.00 10.77	В
	MOTA	4537	CG.	LEU	261	27.276	7.138	51.238	1.00 8.89	В
	MOTA	4538		LEU	261	27.189	5.799	51.975	1.00 7.84	В
	MOTA	4539		LEU	261	27.847	6.973	49.840	1.00 7.48	В
15	MOTA	4540	C	LEU	261	25.993	8.696	53.465	1.00 11.44	В
45	MOTA	4541	0	LEU	261	26.424	9.819	53.247	1.00 13.74	В
	MOTA	4542	N	ASN	262	26.245	8.024	54.586	1.00 10.57	В
	MOTA	4543	CA	asn	262	27.142	8.548	55.615	1.00 8.04	В
	MOTA	4544	CB	ASN	262	26.494	8.386	56.985	1.00 5.60	В
50	MOTA	4545	CG	ASN	262	25.111	8.980	57.011	1.00 B.99	В
50	MOTA	4546	OD1	ASN	262	24.100	8.263	56.971	1.00 9.21	В
	MOTA	4547		ASN	262	25.050	10.307	57.024	1.00 7.62	В
	MOTA	4548	С	ASN	262	28.526	7.879	55.554	1.00 6.87	В
	ATOM	4549	О	ASN	262	28.640	6.653	55.523	1.00 7.74	В
	MOTA	4550	N	LEU	263	29.566	8.705	55.487	1.00 5.79	В
55	MOTA	4551	CA	LEU	263	30.938	8.225	55.438	1.00 5.65	В
	MOTA	4552	CB	LEU	263	31.596	8.741	54.165	1.00 4.90	В
	MOTA	4553	CG	LEU	263	30.735	8.279	52.998	1.00 6.08	В
	ATOM	4554	CD1	LEU	263	31.131	9.012	51.752	1.00 5.33	В
	MOTA	4555		LEU	263	30.853	6.748	52.877	1.00 6.04	В
60	ATOM	4556	C	LEU	263	31.634	8.694	56.710	1.00 6.26	В
	ATOM	4557	0	LEU	263	32.017	9.853	56.842	1.00 B.01	В
	ATOM	4558	N	VAL	264	31.795	7.778	57.653	1.00 6.21	В
	ATOM	4559	CA	VAL	264	32.406	8.079	58.943	1.00 6.25	В
	ATOM	4560	CB	VAL	264	31.600	7.410	60.037	1.00 7.30	В
65	MOTA	4561		VAL	264	32.081	7.848	61.406	1.00 6.21	В
55	ATOM	4562		VAL	264	30.140	7.709	59.802	1.00 0.21	В
	ATOM		C						1.00 7.28	В
	ATOM	4563		VAL	264	33.863	7.677	59.150		
		4564	0	VAL	264	34.221	6.532	58.978	1.00 7.31	В
70	MOTA	4565 4566	N	ASP	265	34.685	8.652	59.533	1.00 9.79	В
,,,	MOTA		CA	ASP	265	36.105	8.441	59.841	1.00 11.34	В
	MOTA	4567	CB	ASP	265	36.978	9.564	59.262	1.00 12.62	В
	ATOM	4568	CC	ASP	265	38.473	9.346	59.520	1.00 16.17	В
	ATOM	4569	001	ASP	265	38.801	8.748	60.562	1.00 17.08	В

	MOTA	4570		ASP	265	39.310	9.783	58.694	1.00 16.43	В
	MOTA	4571	С	ASP	265	36.179	8.527	61.374	1.00 11.75	В
	MOTA	4572	0	ASP	265	36.356	9.601	61.928	1.00 11.74	В
_	MOTA	4573	N	LEU	266	36.032	7.389	62.051	1.00 12.21	В
5	MOTA	4574	CA	LEU	266	36.054	7.367	63.519	1.00 13.54	В
	MOTA	4575	CB	LEU	266	35.692	5.986	64.068	1.00 13.06	В
	MOTA	4576	CG	LEU	266	34.327	5.426	63.711	1.00 14.69	В
	ATOM	4577	CD1	LEU	266	34.190	3.979	64.232	1.00 13.37	В
	MOTA	4578		LEU	266	33.266	6.350	64.285	1.00 14.29	В
10	ATOM	4579	С	LEU	266	37.366	7.763	64.193	1.00 14.66	В
	ATOM	4580	ŏ	LEU	266	38.437	7,776	63.580	1.00 16.77	В
	ATOM	4581	N	ALA	267	37.267	B.097	65.474	1.00 15.57	В
	MOTA	4582	CA	ALA	267	38.435	8.494	66.237	1.00 15.49	В
	MOTA	4583	CB	ALA	267	38.015	9.063	67.584	1.00 15.66	В
15	ATOM	4584	c	ALA	267	39.281	7.256	66.427	1.00 16.90	В.
13	ATOM	4585	ō	ALA	267	38.752	6.166	66.492	1.00 17.09	В
	ATOM	4586	N	GLY	268	40.594	7.432	66.535	1.00 18.45	В
	ATOM	4587	CA	GLY	268	41.470	6.286	66.684	1.00 19.06	В
				GLY	268	40.979	5.375	67.779	1.00 20.29	В
20	ATOM	4588	C	GLY	268	40.476		68.778		В
20	MOTA	4589	0				5.846		1.00 22.63	
	MOTA	4590	N	SER	269	41.153	4.070	67.608	1.00 21.30	В
	ATOM	4591	CA	SER	269	40.683	3.127	68.611	1.00 21.55	В
	ATOM	4592	CB	SER	269	40.151	1.869	67.940	1.00 19.85	В
25	ATOM	4593	OG	SER	269	41.174	1.230	67.206	1.00 19.77	В
23	ATOM	4594	C	SER	269	41.696	2.703	69.666	1.00 23.07	В
	ATOM	4595	0	SER	269	41.415	1.832	70.461	1.00 23.77	. B
	MOTA	4596	N	GLU	270	42.863	3.336	69.682	1.00 24.72	В
	ATOM	4597	CA	GLU	270	43.889	2.997	70.666	1.00 26.45	В
20	ATOM	4598	CB	GLU	270	45.255	3.538	70.212	1.00 26.88	В
30	ATOM	4599	CG	GLU	270	45.365	5.074	70.179	1.00 26.65	В
	ATOM	4600	CD	GLU	270	44.769	5.716	68.938	1.00 25.63	В
	MOTA	4601		GLU	270	44.782	6.966	68.848	1.00 25.90	В
	MOTA	4602	OE2	GLU	270	44.299	4.966	68.063	1.00 25.37	В
25	ATOM	4603	С	GLU	270	43.595	3.501	72.096	1.00 28.21	В
35	MOTA	4604	0	GLU	270	43.182	4.646	72.317	1.00 27.82	В
	ATOM	4605	N	ASN	271	43.804	2.619	73.066	1.00 31.11	В
	ATOM	4606	CA	ASN	271	43.590	2.932	74.483	1.00 33.53	В
	ATOM	4607	CB	ASN	271	42.239	3.620	74.720	1.00 35.28	В
	ATOM	4608	CC	ASN	271	41.046	2.755	74.319	1.00 37.15	В
40	MOTA	4609	OD1	ASN	271	39.892	3.159	74.481	1.00 37.89	В
	MOTA	4610	ND2	ASN	271	41.319	1.569	73.789	1.00 38.13	В
	ATOM	4611	С	ASN	271	43.617	1.669	75.326	1.00 34.61	В
	ATOM	4612	0	ASN	271	43.637	0.561	74.789	1.00 35.03	В
	MOTA	4613	N	ASN	287	41.713	11.898	79.742	1.00 41.72	В
45	ATOM	4614	CA	ASN	287	40.726	12.291	78.737	1.00 42.10	В
	ATOM	4615	CB	ASN	287	41.389	13.166	77.666	1.00 43.36	В
	ATOM	4616	CG	ASN	287	42.137	14.334	78.263	1.00 44.01	В
	ATOM	4617	OD1		287	43.107	14.144	78.990	1.00 44.40	В
	MOTA	4618	ND2		287	41.688	15.548	77.967	1.00 44.56	В
50	ATOM	4619	c	ASN	287	40.094	11.054	78.083	1.00 41.01	В
	ATOM	4620	ō	ASN	287	40.802	10.130	77.661	1.00 42.34	В
	MOTA	4621	N	ILE	288	38.764	11.039	77.994	1.00 37.53	В
	MOTA	4622	CA	ILE	288	38.053	9.905	77.397	1.00 33.20	В
	ATOM	4623	СВ	ILE	288	37.119	9.256	78.433	1.00 33.55	В
55	ATOM	4624	CG2		288	37.940	8.681	79.575	1.00 32.67	В
	ATOM	4625	CG1		288	36.142	10.308	78.967	1.00 33.79	В
	ATOM	4626	CD1		288	35.028	9.764	79.828	1.00 33.79	В
	ATOM	4627				37.221				
			Ç	ILE	288		10.255	76.147 75.946	1.00 29.09 1.00 28.30	В
60	ATOM	4628	0	ILE	288	36.810	11.410			В
00	MOTA	4629	N	ASN	289	36.975	9.258	75.303	1.00 23.27	В
	MOTA	4630	CA	ASN	289	36.172	9.492	74.116	1.00 19.88	В
	MOTA	4631	CB	ASN	289	36.898	B.993	72.871	1.00 18.84	Ð
	MOTA	4632	CG	ASN	289	36.379	9.622	71.601	1.00 19.35	В
65	MOTA	4633	OD1		289	37.155	10.094	70.786	1.00 21.16	В
UJ	ATOM	4634	ND2		289	35.065	9.612	71.415	1.00 18.98	В
	MOTA	4635	C	ASN -		34.829	8.805	74.326	1.00 18.28	В
	ATOM	4636	0	ASN	289	34.628	7.609	74.013	1.00 16.89	В
	MOTA	4637	N	GLN	290	33.906	9.579	74.884	1.00 16.97	В
70	MOTA	4638	CA	CLN	290	32.560	9.115	75.178	1.00 14.08	В
70	MOTA	4639	CB	GLN	290	31.741	10.277	75.738	1.00 15.20	В
	ATOM	4640	CG	GLN	290	30.328	9.905	76.161	1.00 16.32	В
	MOTA	4641	CD	GLN	290	30.274	8.855	77.266	1.00 16.30	В
	MOTA	4642	OE1	GLN	290	29.232	8.273	77.512	1.00 16.57	B

	MOTA	4643	NE2	GLN	290	31.401	8.621	77.934	1.00 17.40	В
	MOTA	4644	С	GLN	290	31.856	8.520	73.959	1.00 12.46	B
	MOTA	4645	0	GLN	290	31.207	7.500	74.055	1.00 12.26	В
-	MOTA	4646	N	SER	291	31.971	9.174	72.814	1.00 11.04	В
5	MOTA	4647	CA	SER	291	31.333	8.627	71.629	1.00 11.96	В
	MOTA	4648	CB	SER	291	31.404	9.609	70.466	1.00 11.35	В
	MOTA	4649	OG	SER	291	30.393	10.586	70.582	1.00 12.37	В
	MOTA	4650	C	SER	291	31.950	7.299	71.201	1.00 11.18	B B
10	MOTA	4651	0	SER	291	31.241 33.270	6.375 7.205	70.783 71.294	1.00 11.32	B
10	ATOM	4652	N	LEU	292	33.965	5.984	70.919	1.00 11.36	В
	ATOM ATOM	4653 4654	CA CB	LEU	292 292	35.485	6.237	70.902	1.00 9.67	В
	ATOM	4655	CG	LEU	292	36.263	5.054	70.334	1.00 10.97	В
	MOTA	4656		LEU	292	35.817	4.822	68.911	1.00 10.21	В
15	MOTA	4657		LEU	292	37.750	5.328	70.387	1.00 13.35	В
	ATOM	4658	c	LEU	292	33.574	4.877	71.914	1.00 11.82	В
	MOTA	4659	ō	LEU	292	33.287	3.724	71.527	1.00 11.11	В
	ATOM	4660	N	LEU	293	33.547	5.232	73.194	1.00 8.02	В
	MOTA	4661	CA	LEU	293	33.210	4.295	74.246	1.00 7.35	В
20	MOTA	4662	CB	LEU	293	33.313	5.005	75.596	1.00 5.38	В
	MOTA	4663	CG	LEU	293	34.410	4.587	76.570	1.00 6.04	В
	MOTA	4664		LEU	293	35.605	3.981	75.841	1.00 3.22	В.
	MOTA	4665		LEU	293	34.798	5.808	77.389	1.00 3.25	В
25	MOTA	4666	C	LEU	293	31.802	3.747	74.071	1.00 7.33	·B
25	MOTA	4667	0	LEU	293	31.563	2.550	74.222	1.00 9.04	В
	ATOM	4668	N	THR	294	30.874	4.646	73.775	1.00 8.36	B B
	MOTA	4669	CA	THR	294 294	29.481 28:623	4.283 5.535	73.604 73.600	1.00 6.48 1.00 5.81	В
	ATOM ATOM	4670 4671	CB	THR THR	294	28.889	6.251	74.804	1.00 6.32	В
30	ATOM	4672			294	27.142	5.206	73.570	1.00 4.45	В
50	MOTA	4673	C	THR	294	29.237	3.461	72.364	1.00 7.94	В
	ATOM	4674	ŏ	THR	294	28.357	2.602	72.368	1.00 9.76	В
	ATOM	4675	N	LEU	295	30.016	3.706	71.310	1.00 6.67	В
	ATOM	4676	CA	LEU	295	29.896	2.918	70.074	1.00 6.68	В
35	MOTA	-4677	CB	LEU	295	30.931	3.313	69.016	1.00 6.59	В
	MOTA	4678	CG	LEU	295	30.897	2.510	67.708	1.00 5.44	В
	MOTA	4679		LEU	295	29.555	2.668	67.036	1.00 4.15	В
	MOTA	4680		LEU	295	31.969	2.993	66.786	1.00 5.26	В
40	MOTA	4681	С	LEU	295	30.228	1.473	70.403	1.00 8.24	В
40	MOTA	4682	0	LEU	295	29.615	0.555	69.887	1.00 9.80	В
	MOTA	4683	N	GLY	296	31.214	1.290	71.276	1.00 9.60	B B
	MOTA MOTA	4684	CA	GLY	296	31.611	-0.047 -0.728	71.669 72.518	1.00 10.99 1.00 12.56	8
	MOTA	4685 4686	С 0	GLY GLY	296 296	30.551 30.275	-1.924	72.350	1.00 12.84	В
45	ATOM	4687	N	ARG	297	29.954	0.037	73.426	1.00 12.22	В
10	MOTA	4688	CA	ARG	297	28.928	-0.486	74.307	1.00 12.41	В
	ATOM	4689	CB	ARG	297	28.692	0.466	75.478	1.00 11.73	В
	MOTA	4690	CG	ARG	297	29.818	0.493	76.498	1.00 10.69	B
	MOTA	4691	CD	ARG	297	29.767	1.736	77.378	1.00 11.84	В
50	ATOM	4692	NE	ARG	297	30.969	1.856	78.205	1.00 10.74	В
	MOTA	4693	CZ	ARG	297	31.409	2.993	78.734	1.00 10.49	В
	MOTA	4694		ARG	297	30.743	4.119	78.517	1.00 11.64	В
	MOTA	4695		ARG.		32.504	3.003	79.486	1.00 9.73	В
55	MOTA	4696	c	ARG	297	27.622	-0.708	73.569	1.00 13.86 1.00 13.06	B B
55	ATOM	4697	O N	ARG VAL	297 298	26.798 27.426	-1.514 0.014	74.009 72.464	1.00 14.33	В
	MOTA MOTA	4698 4699	CA	VAL	298	26.216	-0.134	71.659	1.00 16.21	В
	MOTA	4700	CB	VAL	298	26.048	1.031	70.696	1.00 16.05	В.
	ATOM	4701		VAL	298	25.021	0.679	69.639	1.00 17.88	B
60	ATOM	4702		VAL	298	25.605	2,257	71.458	1.00 18.13	B
	ATOM	4703	c	VAL	298	26.281	-1.426	70.853	1.00 17.16	В
	MOTA	4704	ō	VAL	298	25.305	-2.173	70.774	1.00 18.74	В
	ATOM	4705	N	ILE	299	27.441	-1.691	70.262	1.00 18.24	В
	ATOM	4706	CA	ILE	299	27.645	-2.910	69.486	1.00 18.96	В
65	MOTA	4707	CB	ILE	299	29.019	-2.868	68.770	1.00 19.68	В
	ATOM	4708		ILE	299	29.368	-4.245	68.184	1.00 17.64	В
	MOTA	4709		ILE	299	28.983	-1.791	67.674	1.00 19.70	В
	MOTA	4710		ILE	299	30.314	-1.589	66.977	1.00 22.74	В
70	MOTA	4711	C	ILE	299	27.551	-4.142	70.400	1.00 19.56	В
70	MOTA	4712	0	ILE	299	27.027	-5.191	70.012	1.00 19.03	В
	ATOM	4713	N	THR	300	28.043	-4.017	71.624	1.00 19.86	В
	MOTA	4714	CA	THR	300	27.978	-5.136	72.551	1.00 20.92 1.00 20.58	B B
	MOTA	4715	CB	THR	300	28.770	-4.841	73.824	1.00 20.58	

	ATOM	4716	0G1	THR	300	30.172	-4.893	73.533	1.00 21.97	В
	MOTA	4717	CG2		300	28.433	-5.845	74.903	1.00 21.65	В
	MOTA	4718	c	THR	300	26.525	-5.450	72.915	1.00 21.71	В
	ATOM	4719	ō	THR	300	26.134	-6.601	72.984	1.00 22.71	В
5				ALA	301	25.728	-4.413	73.139	1.00 23.13	В
5	MOTA	4720	N					73.494	1.00 23.01	В
	MOTA	4721	CA	ALA	301	24.337	-4.624		1.00 22.73	В
	ATOM	4722	CB	ALA	301	23.694	-3.327	73.904		В
	MOTA	4723	С	ALA	301	23.589	-5.225	72.323	1.00 23.48	
10	ATOM	4724	0	ALA	301	22.652	-5.982	72.509	1.00 23.63	В
10	MOTA	4725	N	LEU	302	24.005	-4.872	71.111	1.00 23.21	В
	MOTA	4726	CA	LEU	302	23.361	-5.392	69.911	1.00 24.59	В
	MOTA	4727	CB	LEU	302	23.737	-4.526	68.695	1.00 23.93	В
	MOTA	4728	CG	LEU	302	22.774	-3.511	68.059	1.00 22.99	В
	ATOM	4729	CD1	LEU	302	21.827	-2.952	69.058	1.00 20.71	В
15	ATOM	4730	CD2	LEU	302	23.579	-2.394	67.440	1.00 21.49	В
	ATOM	4731	С	LEU	302	23.728	-6.861	69.656	1.00 25.70	В
	ATOM	4732	ō	LEU	302	22.847	-7.695	69.406	1.00 24.83	В
	MOTA	4733	N	VAL	303	25.021	-7.170	69.731	1.00 27.74	В
	MOTA	4734	Ċλ	VAL	303	25.527	-8.521	69.505	1.00 29.35	В
20	ATOM	4735	CB	VAL	303	27.054	-8.549	69.593	1.00 29.55	В
20	MOTA	4736		VAL	303	27.545	-9.975	69.439	1.00 30.49	В
			CG2		303	27.651	-7.641	68.524	1.00 30.24	В
	ATOM	4737						70.510	1.00 31.00	В
	MOTA	4738	C	VAL	303	24.985	-9.528	70.310	1.00 30.43	В
25	ATOM	4739	0	VAL	303	24.629	-10.631		1.00 33.86	В
23	ATOM	4740	N	GLU	304	24.927	-9.123	71.770		В
	MOTA	4741	CA	GLU	304	24.442	-9.986	72.838	1.00 36.40	
	ATOM	4742	CB	GLU	304	25.130	-9.594	74.143	1.00 37.33	В
	ATOM	4743	CG	GLU	304	26.650	-9.690	74.076	1.00 39.18	В
~~	MOTA	4744	CD	GLU	304	27.316	-9.437	75.422	1.00 41.19	В
30	MOTA	4745	0E1	GLU	304	28.564	-9.473	75.490	1.00 42.27	В
	MOTA	4746	OE2	GLU	304	26.594	-9.202	76.413	1.00 42.10	В
	MOTA	4747	С	GLU	304	22.922	-9.924	72.985	1.00 38.11	В
	MOTA	4748	0	GLU	304	22.334	-10.552	73.871	1.00 37.60	В
	ATOM	4749	N	ARG	305	22.303	-9.155	72.098	1.00 41.03	В
35	MOTA	4750	CA	ARG	305	20.860	-8.996	72.068	1.00 43.26	В
	ATOM	4751	CB	ARG	305	20.221	-10.302	71.592	1.00 44.67	В
	ATOM	4752	CG	ARG	305		-10.629	70.151	1.00 46.86	· B
	MOTA	4753	CD	ARG	305		-12.025	69.716	1.00 49.68	В
	ATOM	4754	NE	ARG	305		-12.350	68.373	1.00 50.79	В
40	ATOM	4755	cz	ARG	305		-11.753	67.258	1.00 50.97	В
-10	ATOM	4756		ARG	305		-10.797	67.309	1.00 51.47	В
		4757		ARG	305		-12.097	66.089	1.00 51.54	В
	MOTA				305	20.237	-8.514	73.367	1.00 43.49	В
	MOTA	4758	c	ARG		19.142	-8.909	73.718	1.00 44.11	В
45	MOTA	4759	0	ARG	305				1.00 44.17	В
43	MOTA	4760	N	THR	306	20.951	-7.648	74.077		В
	ATOM	4761	CA	THR	306	20.444	-7.078	75.319	1.00 43.76	
	MOTA	4762	CB	THR	306	21.535	-6.267	76.040	1.00 43.72	В
	MOTA	4763		THR	306	22.623	-7.131	76.399	1.00 43.84	В
50	MOTA	4764		THR	306	20.975	-5.602	77.288	1.00 43.30	В
50	MOTA	4765	С	THR	306	19.307	-6.139	74.912	1.00 44.17	В
	MOTA	4766	0	THR	306	19.388	-5.459	73.891	1.00 45.09	В
	MOTA	4767	N	PRO	307	18.226	-6.098	75.700	1.00 43.54	В
	MOTA	4768	CD	PRO	307	17.925	-6.973	76.846	1.00 43.66	В
	MOTA	4769	CA	PRO	307	17.080	-5.232	75.390	1.00 42.75	В
55	MOTA	4770	CB	PRO	307	16.101	-5.554	76.518	1.00 43.35	В
	ATOM	4771	CG	PRO	307	16.429	-7.001	76.834	1.00 44.16	В
	MOTA	4772	c	PRO	307	17.408	-3.741	75.269	1.00 41.65	В
	MOTA	4773	ŏ	PRO	307	16.903	-3.049	74.384	1.00 41.15	В
	MOTA	4774	N	HIS	308	18.254	-3.247	76.166	1.00 39.72	В
60	MOTA	4775	CA	HIS	308	18.629	-1.839	76.164	1.00 37.51	В
00					308	18.774	-1.336	77.587	1.00 39.81	В
	MOTA	4776	CB	HIS			0.097		1.00 42.26	В
	MOTA	4777	CG	HIS	308	19.193		77.677		В
	MOTA	4778		HIS	308	20.336	0.664	78.127	1.00 43.26	
65	MOTA	4779		HIS	308	18.391	1.131	77.247	1.00 43.54	В
65	MOTA	47B0		HIS	308	19.024	2.278	77.428	1.00 44.49	В
	MOTA	4781		HIS	308	20.205	2.024	77.959	1.00 44.29	В
	MOTA	4782	С	HIS	308	19.937	-1.559	75.446	1.00 35.63	В
	MOTA	4783	0	HIS	308	20.958	-2.160	75.745	1.00 36.69	В
	ATOM	4784	N	VAL	309	19.889	-0.627	74.501	1.00 32.04	В
70	MOTA	4785	CA	VAL	309	21.071	-0.237	73.731	1.00 27.44	В
	ATOM	4786	CB	VAL	309	20.821	-0.415	72.218	1.00 27.23	В
	MOTA	4787		VAL	309	22.090	-0.111	71.426	1.00 27.83	В
	ATOM	4788		VAL	309	20.336	-1.823	71.946	1.00 25.00	В
	011									

	ATOM	4789	С	VAL	309	21.307	1.234	74.059	1.00 26.45	В
	MOTA	4790	0	VAL	309	20.501	2.090	73.724	1.00 26.41	В
	ATOM	4791	N	PRO	310	22.432	1.538	74.715	1.00 25.12	В
	ATOM	4792		PRO	310	23.508	0.587	75.062	1.00 23.57	В
5										
3	MOTA	4793	CA	PRO	310	22.780	2.914	75.107	1.00 22.73	В
	MOTA	4794	CB	PRO	310	23.985	2.701	76.007	1.00 23.56	В
							1.504		1.00 23.96	В
	ATOM	4795		PRO	310	24.671		75.354		
	ATOM	4796	С	PRO	310	23.017	3.958	73.999	1.00 22.22	В
	ATOM	4797	0	PRO	310	23.965	4.735	74.073	1.00 21.14	В
10										
10	MOTA	4798		TYR	311	22.147	4.000	72.995	1.00 21.70	В
	ATOM	4799	·CA	TYR	311	22.294	4.967	71.899	1.00 22.33	В
	ATOM	4800		TYR	311	21.083	4.978	70.970	1.00 22.30	В
	ATOM	4801	CG	TYR	311	20.861	3.721	70.154	1.00 24.68	В
	ATOM	4802	CD1	TYR	311	21.773	3.322	69.177	1.00 25.08	В
- 15							2.171	68.411	1.00 25.18	В
. 13	ATOM	4803		TYR	311	21.555				
	ATOM	4804	CD2	TYR	311	19.717	2.937	70.347	1.00 24.09	В
	ATOM	4805	CE2	TYR	311	19.493	1.786	69.590	1.00 24.09	В
					• .					
	ATOM	4806		TYR	311	20.416	1.405	68.623	1.00 24.98	В
	MOTA	4807	OH '	TYR	311	20.211	0.246	67.893	1.00 24.66	В
20	ATOM	4808	C	TYR	311	22.431	6.429	72.338	1.00 21.98	В
										В
	MOTA	4809		TYR	311	23.180	7.188	71.741	1.00 23.57	
	ATOM	4810	N .	ARG	312	21.707	6.813	73.384	1.00 20.49	В.
	MOTA	4811	CA	ARG	312	21.726	8.203	73.861	1.00 19.38	В
25	MOTA	4812		ARG	312	20.447	8.544	74.640	1.00 21.56	· B
25	MOTA	4813	CG	ARG	312	19.150	8.149	73.951	1.00 24.98	В
	MOTA	4814	CD .	ARG	312	17.949	8.887	74.534	1.00 27.94	В
	MOTA	4815		ARG	312	16.688	8.240	74.175	1.00 31.63	В
	MOTA	4816	CZ.	ARG	312	16.262	7.086	74.688	1.00 34.10	В
	ATOM	4817	NH1		312	16.996	6.445	75.590	1.00 37.15	В
30										
30	MOTA	4818	NH2	ARG	312	15.101	6.566	74.304	1.00 33.60	В
	ATOM	4819	C .	ARG	312	22.875	8.612	74.779	1.00 17.27	В
	ATOM	4820		ARG	312	22.933	9.756	75.235	1.00 16.64	В
	MOTA	4821	N	GLU	313	23.786	7.686	75.054	1.00 14.25	В
	MOTA	4822	CA	GLU	313	24.908	7.986	75.935	1.00 11.55	В
35	ATOM	4823		GLU	313	25.410	6.693	76.590	1.00 11.14	В
55										
	MOTA	4824	CG	GLU	313	24.416	6.136	77.618	1.00 11.41	В
	ATOM	4825	CD	GLU	313	24.916	4.905	78.379	1.00 12.57	В
	ATOM	4826	OE1			26.071	4.898	78.834	1.00 11.41	В
					313					
	MOTA	4827	OE2	GLU	313	24.149	3.935	78.569	1.00 14.80	В
40	MOTA	4828	C	GLU	313	26.053	8.746	75.271	1.00 10.23	В
										В
	ATOM	4829		CLU	313	27.066	8.960	75.891	1.00 10.15	
	MOTA	4830	N	SER	314	25.865	9.164	74.017	1.00 10.36	В
	ATOM	4831	CA	SER	314	26.878	9.912	73.263	1.00 9.41	В
45	ATOM	4832		SER	314	28.000	9.018	72.732	1.00 10.81	В
45	ATOM	4833	OG	SER	314	27.643	8.320	71.544	1.00 9.64	В
	ATOM	4834	C	SER	314	26.235	10.511	72.031	1.00 10.05	В
	ATOM	4835	0.	SER	314	25.190	10.052	71.583	1.00 9.18	В
	ATOM	4836	N	LYS	315	26.887	11.544	71.501	1.00 10.81	В
	ATOM	4837		LYS	315	26.428	12.259	70.320	1.00 9.07	В
50										
50	MOTA	4838	CB	LYS	315	27.254	13.527	70.063	1.00 9.50	В
	MOTA	4839	CG	LYS	315	27.390	14.463	71.236	1.00 9.25	В
	MOTA	4840		LYS	315	26.058	14.973	71.686	1.00 10.89	В
	MOTA	4841	CE	LYS	315	26.244	16.156	72.620	1.00 13.02	B
	ATOM	4842	NZ	LYS	315	26.918	17.316	71.937	1.00 14.10	В
55	ATOM	4843		LYS	315	26.556	11.414	69.077	1.00 8.68	В
45										
	MOTA	4844	0	LYS	315	25.652	11.383	68.282	1.00 10.14	В
	MOTA	4845	N	LEU	316	27.683	10.721	68.931	1.00 8.28	B
	MOTA	4846		LEU	316	27.928	9.888	67.763	1.00 7.48	В.
	ATOM	4847	CB	LEU	316	29.297	9.205	67.867	1.00 6.90	В
60	ATOM	4848	CG	LEU	316	29.679	8.277	66.713	1.00 8.06	В
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	ATOM	4849	CD1		316	30.018	9.097	65.484	1.00 10.24	В
	MOTA	4850	CD2	LEU	316	30.850	7.452	67.129	1.00 8.22	В
	MOTA	4851		LEU	316	26.852	8.821	67.590	1.00 9.38	В
15	MOTA	4852		LEU	316	26.241	8.733	66.523	1.00 9.82	В
65	MOTA	4853	N	THR	317	26.588	8.040	68.642	1.00 9.80	В
-	ATOM	4854				25.599	6.965	68.534	1.00 10.18	В
				THR	317					
	MOTA	4855	CB '	THR	317	25.672	5.952	69.674	1.00 10.15	В
	ATOM	4856	0G1 '		317	25.527	6-642	70.909	1.00 10.81	В
70	ATOM	4857	CGS		317	27.004	5.185	69.661	1.00 9.59	В
70	ATOM	4858	C '	THR	317	24.175	7.455	68.484	1.00 10.03	В
	ATOM	4859		THR	317	23.295	6.709	68.146	1.00 11.71	В
	ATOM	4860		ARG	318	23.947	8.703	68.867	1.00 9.69	В
	ATOM	4861	CA .	ARG	318	22.607	9.256	68.785	1.00 9.04	В
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	MOTA	4862	CB	ARG	318	22.454	10.464	69.703	1.00 13.23	В
	MOTA	4863	CG	ARG	318	21.719	10.147	71.004	1.00 19.08	В
	MOTA	4864	CD	ARG	318	22.058	11.133	72.115	1.00 22.73	В
	ATOM	4865	NE	ARG	318	21.617	12.495	71.828	1.00 26.31	B
5	MOTA	4866	CZ	ARG	318	20.345	12.863	71.705	1.00 27.29	В
-	ATOM	4867	NH1		318	19.383	11.963	71.849	1.00 28.67	В
	ATOM	4868	NH2		318	20.036	14.124	71.429	1.00 25.94	В
	ATOM	4869	C	ARG	318	22.434	9.679	67.344	1.00 8.51	В
	MOTA	4870	ŏ	ARG	318	21.418	9.412	66.720	1.00 10.84	В
10	MOTA	4871	N	ILE	319	23.445	10.339	66.799	1.00 5.66	B
10	ATOM	4872	CA	ILE	319	23.352	10.766	65.410	1.00 5.05	В
					319	24.591		65.014	1.00 5.19	В
	MOTA	4873	CB	ILE			11.627			B
	MOTA	4874		ILE	319	24.531	11.976	63.544	1.00 6.51	
15	ATOM	4875		ILE	319	24.603	12.935	65.826	1.00 5.47	В
13	ATOM	4876		ILE	319	25.833	13.774	65.632	1.00 2.71	В
	MOTA	4877	C	ILE	319	23.227	9.551	64.460	1.00 3.03	В
	MOTA	4878	0	ILE	319	22.361	9.511	63.590	1.00 1.95	В
	MOTA	4879	N	LEU	320	24.067	8.540	64.657	1.00 4.41	₿
20	MOTA	4880	CA	LEU	320	24.056	7.376	63.767	1.00 5.60	₽
20	MOTA	4881	СВ	LEU	320	25.490	6.931	63.451	1.00 2.81	В
	MOTA	4882	CG	LEU	320	26.437	7.964	62.845	1.00 2.57	В
	ATOM	4883		LEU	320	27.873	7.442	62.786	1.00 2.20	В
	MOTA	4884	CD2	LEU	320	25.955	8.334	61.476	1.00 1.00	В
	ATOM	4885	С	LEU	320	23.313	6.122	64.235	1.00 7.52	В
25	MOTA	4886	0	LEU	320	23.620	5.045	63.776	1.00 7.94	В
	MOTA	4887	N	GLN	321	22.306	6.258	65.094	1.00 10.60	. В
	MOTA	4888	CA	GLN	321	21.629	5.057	65.604	1.00 16.44	В
	MOTA	4889	CB	GLN	321	20.679	5.362	66.775	1.00 18.94	В
	ATOM	4890	CG	GLN	321	19.433	6.153	66.458	1.00 22.43	В
30	ATOM	4891	CD	GLN	321	18.593	6.391	67.707	1.00 25.16	В
	ATOM	4892		GLN	321	18.121	5.453	68.338	1.00 26.09	В
	ATOM	4893	NE2		321	18.418	7.658	68.071	1.00 26.05	B
	ATOM	4894	C	GLN	321	20.882	4.186	64.617	1.00 16.64	В
	ATOM	4895	ŏ	GLN	321	20.700	2.992	64.870	1.00 16.23	В
35	MOTA	4896	N	ASP	322	20.439	4.759	63.505	1.00 17.01	В
-	ATOM	4897	CA	ASP	322	19.762	3.931	62.521	1.00 19.03	В
	MOTA	4898	СВ	ASP	322	18.952	4.755	61.535	1.00 20.75	В
	ATOM	4899	cc	ASP	322	17.983	3.896	60.727	1.00 22.50	B
	ATOM	4900		ASP	322	17.835	4.125	59.506	1.00 24.17	В
40	ATOM	4901		ASP	322	17.352	2.997	61.327	1.00 21.00	В
70							3.139	61.722	1.00 20.46	В
	MOTA	4902 4903	C O	ASP ASP	322 322	20.803 20.467	2.335	60.861	1.00 23.04	В
	ATOM						3.385	62.006	1.00 20.16	В
	ATOM	4904	N	SER	323	22.076		61.353	1.00 18.88	В
45	MOTA	4905	CA	SER	323	23.164	2.670			В
73	MOTA	4906	CB	SER	323	24.299	3.643	61.077	1.00 17.96	
	MOTA	4907	OG	SER	323	23.842	4.642	60.187	1.00 18.62	В
	MOTA	4908	С	SER	323	23.625	1.518	62.259	1.00 18.52	В
	ATOM	4909	0	SER	323	24.368	0.647	61.838	1.00 19.83	В
50	MOTA	4910	N	LEU	324	23.168	1.512	63.507	1.00 16.09	В
50	ATOM	4911	CA	LEU	324	23.541	0.449	64.420	1.00 16:61	В
	ATOM	4912	СВ	LEU	324	24.257	1.026	65.648	1.00 15.87	В
	ATOM	4913	CG	LEU	324	25.679	1.595	65.539	1.00 14.59	В
	MOTA	4914		LEU	324	26.545	0.643	64.722	1.00 13.37	В
	ATOM	4915		LEU	324	25.649	2.965	64.909	1.00 11.67	В
55	MOTA	4916	С	LEU	324	22.300	-0.343	64.834	1.00 17.48	В
	MOTA	4917	0	LEU	324	21.651	-0.025	65.814	1.00 16.83	В
	MOTA	4918	N	GLY	325	21.983	-1.387	64.071	1.00 17.97	В
	MOTA	4919	CA	GLY	325	20.818	-2.203	64.377	1.00 18.49	В
	MOTA	4920	С	GLY	325	19.498	-1.576	63.939	1.00 19.29	В
60	MOTA	4921	0	GLY	325	18.427	-1.950	64.423	1.00 19.24	В
	MOTA	4922	N	GLY	326	19.573	-0.630	63.007	1.00 19.01	В
	ATOM	4923	CA	GLY	326	18.382	0.052	62.539	1.00 18.79	В
	MOTA	4924	С	GLY	326	17.935	-0.373	61.165	1.00 19.04	В
	ATOM	4925	ō	GLY	326	17.931	-1.550	60.861	1.00 18.81	В
65	MOTA	4926	N	ARG	327	17.565	0.603	60.341	1.00 19.26	В
	ATOM	4927	CA	ARG	327	17.106	0.336	58.991	1.00 20.71	В
	ATOM	4928	CB	ARG	327	15.731	0.970	58.761	1.00 22.28	В
	MOTA	4929	CG	ARG	327	14.591	0.225	59.443	1.00 25.87	В
	MOTA	4930	CD	ARG	327	13.233	0.703	58.976	1.00 28.38	В
70	MOTA	4931	NE	ARG	327	12.260	-0.388	58.957	1.00 23.33	В
. •	ATOM	4932	CZ	ARG	327	12.200	-1.477	58.193	1.00 36.86	В
	ATOM	4933		ARG			-1.639	57.382	1.00 38.23	В
	ATOM	4934			327	13.412			1.00 38.23	В
	ALON	4734	MH2	ARG	327	11.422	-2.399	58.213	1.00 30.3/	ь

	MOTA	4935	С	ARG	327	18.072	0.784	57.899	1.00 20.64	В
	MOTA	4936	ŏ	ARG	327	17.721	0.788	56.718	1.00 19.55	В
	MOTA	4937	N	THR	328	19.295	1.127	58.293	1.00 19.88	В
					328	20.316	1.568	57.349	1.00 18.38	В
5	MOTA	4938	CA	THR			2.694	57.948	1.00 16.59	В
ر	MOTA	4939	CB	THR	328	21.133				В
	ATOM	4940	OG1		328	20.260	3.780	58.254	1.00 15.01	
	MOTA	4941	CG2		328	22.170	3.171	56.975	1.00 16.39	В
	MOTA	4942	С	THR	328	21.271	0.449	56.971	1.00 17.88	B
	MOTA	4943	0	THR	328	21.640	-0.343	57.808	1.00 18.85	В
10	ATOM	4944	N	ARG	329	21.659	0.380	55.701	1.00 18.85	В
	MOTA	4945	·CA	ARG	329	22.605	-0.648	55.284	1.00 18.48	В
	MOTA	4946	CB	ARG	329	22.644	-0.784	53.756	1.00 21.31	B
	MOTA	4947	CG	ARG	329	23.540	-1.929	53.249	1.00 27.66	В
	MOTA	4948	CD	ARG	329	23.818	-1.771	51,.748	1.00 32.45	В
15	ATOM	4949	NE	ARG	329	24.651	-2.837	51.190	1.00 38.68	В
	ATOM	4950	CZ	ARG	329	25.871	-3.147	51.626	1.00 43.03	В
	MOTA	4951		ARG	329	26.417	-2.475	52.641	1.00 45.11	В
	MOTA	4952	NH2		329	26.553	-4.122	51.032	1.00 45.04	В
	ATOM	4953	C	ARG	329	23.937	-0.161	55.840	1.00 14.99	В
20	ATOM	4954	õ	ARG	329	24.361	0.948	55.568	1.00 16.21	В
LU		4955	N	THR	330	24.595	-0.987	56.632	1.00 12.23	В
	MOTA		CA		330	25.842	-0.559	57.235	1.00 11.36	В.
	MOTA	4956		THR				58.801	1.00 11.85	В.
	MOTA	4957	CB	THR	330	25.720	-0.515	59.185	1.00 12.21	·B
25	MOTA	4958		THR	330	24.663	0.378			В
25	MOTA	4959		THR	330	27.022	-0.038	59.432	1.00 10.17	
	MOTA	4960	C	THR	330	27.031	-1.424	56.857	1.00 11.32	В
	MOTA	4961	0	THR	330	26.909	-2.639	56.699	1.00 11.14	В
	MOTA	4962	N	SER	331	28.176	-0.760	56.722	1.00 10.11	В
20	MOTA	4963	CA	SER	331	29.432	-1.390	56.396	1.00 9.70	В
30	ATOM	4964	CB	SER	331	29.762	-1.121	54.938	1.00 10.15	В
	MOTA	4965	OG	SER	331	29.612	-2.305	54.201	1.00 16.41	В
	MOTA	4966	С	SER	331	30.551	-0.861	57.292	1.00 8.79	В
	ATOM	4967	0	SER	331	30.612	0.314	57.575	1.00 10.25	В
	MOTA	4968	N	ILE	332	31.421	-1.744	57.761	1.00 7.54	В
35	MOTA	.4969	CA	ILE	332	32.537	-1.309	58.580	1.00 5.00	В
	MOTA	4970	СВ	ILE	332	32.484	-1.896	59.997	1.00 3.72	В
	MOTA	4971	CG2	ILE	332	33.791	-1.623	60.719	1.00 1.00	В
	ATOM	4972		ILE	332	31.296	-1.308	60.755	1.00 1.20	В
	ATOM	4973		ILE	332	31.044	-1.996	62.080	1.00 1.00	В
40	ATOM	4974	c	ILE	332	33.825	-1.761	57.915	1.00 6.57	В
	ATOM	4975	ŏ	ILE	332	33.959	-2.921	57.505	1.00 6.08	В
	MOTA	4976	N	ILE	333	34.754	-0.824	57.779	1.00 6.74	В
	MOTA	4977	CA	ILE	333	36.052	-1.110	57.203	1.00 7.94	В
		4978	CB	ILE	333	36.377	-0.134	56.043	1.00 7.86	В
45	MOTA					37.745	-0.446	55.482	1.00 10.20	В
45	ATOM	4979		ILE	333				1.00 9.26	В
	MOTA	4980		ILE	333	35.335	-0.292	54.935		В
	MOTA	4981		ILE	333	35.562	0.532	53.743		В
	MOTA	4982	С	ILE	333	37.050	-0.961	58.362	1.00 9.22	
50	MOTA	4983	0	ILE	333	37.318	0.139	58.833	1.00 9.93	В
50	MOTA	4984	N	ALA	334	37.568	-2.087	58.842	1.00 9.27	В
	ATOM	4985	CA	ALA	334	38.510	-2.064	59.950	1.00 9.36	В
	MOTA	4986	CB	ALA	334	38.318	-3281	60.815	1.00 8.99	В
	MOTA	4987	С	ALA	334	39.914	-2.033	59.366	1.00 9.97	В
	MOTA	4988	0	ALA	334	40.289	-2.887	58.558	1.00 9.97	B
55	MOTA	4989	N	THR	335	40.689	-1.039	59.780	1.00 10.59	В
	MOTA	4990	CA	THR	335	42.041	-0.877	59.267	1.00 11.33	В
	MOTA	4991	CB	THR	335	42.300	0.587	58.833	1.00 11.54	В
	ATOM	4992	0G1	THR	335	42.165	1.471	59.959	1.00 11.31	В
	MOTA	4993	CG2	THR	335	41.316	0.973	57.707	1.00 10.89	В
60	MOTA	4994	c	THR	335	43.059	-1.311	60.297	1.00 11.80	В
••	MOTA	4995	ŏ	THR	335	42.898	-1.044	61.479	1.00 11.91	В
	MOTA	4996	N	ILE	336	44.108	-1.981	59.825	1.00 10.99	В
		4990		ILE	336	45.150	-2.494	60.691	1.00 9.23	В
	MOTA	4998	CA				-4.002	60.867	1.00 6.21	B
65	MOTA		CB	ILE	336	44.988			1.00 2.30	В
U)	MOTA	4999		ILE	336	43.726	-4.275	61.631		В
	MOTA	5000		ILE	336	44.949	-4.688	59.501	1.00 4.99	
	MOTA	5001		ILE	336	44.977	-6.187	59.570	1.00 4.80	В
	MOTA	5002	С	ILE	336	46.549	-2.201	60.175	1.00 12.29	В
70	MOTA	5003	0	ILE	336	46.722	-1.683	59.054	1.00 12.52	B
70	MOTA	5004	N	SER	337	47.536	-2.533	61.011	1.00 15.10	В
	MOTA	5005	CA	SER	337	48.958	-2.344	60.716	1.00 17.38	В
	MOTA	5006	CB-	SER	337	49.673	-1.619	61.848	1.00 16.32	В
	MOTA	5007	OG	SER	337	51.071	-1.842	61.757	1.00 15.90	В

	ATOM	5008	С	SER	337	49.690	-3.686	60.569	1.00 18.53	В
	MOTA	5009	ō	SER	337	49.393	-4.652	61.292	1.00 19.54	В
	MOTA	5010	N	PRO	338	50.643	-3.770	59.618	1.00 17.27	В
					338		-2.790	58.555	1.00 15.95	В
5	MOTA	5011	CD	PRO		50.949.				В
,	MOTA	5012	CA	PRO	338	51.398	-5.005	59.403	1.00 15.90	
	MOTA	5013	CB	PRO	338	51.851	-4.868	57.953	1.00 14.63	В
	ATOM	5014	CG	PRO	338	52.158	-3.420	57.858	1.00 15.30	В
	MOTA	5015	С	PRO	338	52.574	-5.124	60.360	1.00 15.45	В
	MOTA	5016	0	PRO	338	53.206	-6.145	60.420	1.00 15.18	В
10	ATOM	5017	N	ALA	339	52.844	-4.053	61.103	1.00 16.79	В
	MOTA	5018	CA	ALA	339	53.986	-3.999	62.025	1.00 19.03	В
						54.296	-2.536	62.409	1.00 17.80	В
	MOTA	5019	CB	ALA	339				1.00 17.00	
	ATOM	5020	C	ALA	339	53.813	-4.824	63.277		В
1.0	MOTA	5021	0	ALA	339	52.727	-4.883	63.824	1.00 21.39	В
15	MOTA	5022	N	SER	340	54.896	-5.452	63.734	1.00 20.20	В
	MOTA	5023	CA	SER	340	54.825	-6.278	64.940	1.00 20.54	В
	MOTA	5024	CB	SER	340	56.045	-7.193	65.075	1.00 21.46	В
	MOTA	5025	OG	SER	340	57.233	-6.430	65.182	1.00 24.93	B
	ATOM	5026	C	SER	340	54.727	-5.453	66.208	1.00 19.22	В
20	ATOM	5027	ŏ	SER	340	54.293	-5.941	67.224	1.00 17.09	В
	MOTA	5028	N	LEU	341	55.131	-4.191	66.143	1.00 20.29	В
									1.00 21.64	В
	ATOM -	5029	CA	LEU	341	55.048	-3.345	67.328		В
	MOTA	5030	CB	LEU	341	56.040	-2.184	67.248	1.00 23.99	
25	MOTA	5031	CG	LEU	341	55.610	-0.896	66.546	1.00 27.23	В
25	ATOM	5032	CD1	LEU	341	55.641	0.269	67.554	1.00 26.67	В
	MOTA	5033	CD2	LEU	341	56.542	-0.630	65.357	1.00 28.22	В
	MOTA	5034	С	.LEU	341	53.629	-2.807	67.502	1.00 21.40	В
	MOTA	5035	0	LEU	341	53.350	-2.053	68.424	1.00 21.64	В
	MOTA	5036	N	ASN	342	52.736	-3.227	66.613	1.00 21.16	В
30	MOTA	5037	CA	ASN	342-	51.335	-2.815	66.664	1.00 21.98	В
20			CB	ASN	342	50.943	-2.165	65.352	1.00 20.54	В
	MOTA	5038		ASN						В
	MOTA	5039	CG		342	51.586	-0.826	65.172	1.00 21.64	
	MOTA	5040		ASN	342	51.897	-0.423	64.046	1.00 19.82	В
25	ATOM	5041		ASN	342	51.785	-0.107	66.285	1.00 20.76	В
35	MOTA	5042	С	ASN	342	50.415	-4.011	66.892	1.00 22.33	В
	MOTA	5043	0	ASN	342	49.201	-3.909	66.761	1.00 22.21	В
	ATOM	5044	N	LEU	343	51.023	~5.135	67.254	1.00 23.56	В
	MOTA	5045	CA	LEU	343	50.334	-6.406	67.488	1.00 24.35	В
	ATOM	5046	СВ	LEU	343	51.360	-7.435	67.992	1.00 25.91	В
40	ATOM	5047	CG	LEU	343	50.986	-8.890	68.316	1.00 28.30	В
70						50.524	-8.995	69.761	1.00 29.51	B
	MOTA	5048		LEU	343					В
	MOTA	5049		LEU	343	49.930	-9.392	67.334	1.00 28.29	
	MOTA	5050	С	LEU	343	49.119	-6.347	68.412	1.00 22.80	В
40	MOTA	5051	0	LEU	343	48.024	-6.756	68.045	1.00 21.40	В
45	ATOM	5052	N	GLU	344	49.305	-5.831	69.614	1.00 23.08	В
	MOTA	5053	CA	GLU	344	48.189	-5.745	70.545	1.00 22.34	В
	ATOM	5054	CB	GLU	344	48.628	-5.122	71.861	1.00 24.68	В
	MOTA	5055	CG	GLU	344	47.491	-4.875	72.821	1.00 30.10	В
	ATOM	5056	CD	GLU	344	47.965	-4.715	74.263	1.00 34.59	В
50	MOTA	5057		GLU	344	48.866	-3.886	74.538	1.00 36.85	В
50	ATOM	5058		GLU	344	47.422	-5.428	75.134	1.00 36.33	В
							-4.960	70.002	1.00 19.86	В
	MOTA	5059	c	GLU	344	47.002			1.00 20.25	В
	MOTA	5060	0	GLU	344	45.894	-5.425	70.097		
<i>C C</i>	MOTA	5061	N	GLU	345	47.241	-3.770	69.452	1.00 17.13	В
55	MOTA	5062	CA	CLU	345	46.141	-2.974	68.907	1.00 16.35	В
	MOTA	5063	CB	GLU	345	46.585	-1.527	68.589	1.00 15.68	В
	MOTA	5064	CG	GLU	345	46.803	-0.645	69.824	1.00 13.57	В
	MOTA	5065	CD	GLU	345	45.528	-0.391	70.618	1.00 13.00	В
	MOTA	5066		GLU	345	45.623	0.062	71.768	1.00 14.32	В
60 ·	ATOM	5067		GLU	345	44.419	-0.628	70.111	1.00 13.44	В
00				GLU						В
	MOTA	5068	C		345	45.528	-3.626	67.659	1.00 14.78	
	MOTA	5069	0	GLU	345	44.326	-3.544	67.442	1.00 14.79	В
	MOTA	5070	N	THR	346	46.350	-4.284	66.846	1.00 14.54	В
15	MOTA	5071	CA	THR	346	45.863	-4.959	65.641	1.00 14.71	В
65	MOTA	5072	CB	THR	346	47.046	-5.572	64.839		В
	MOTA	5073	0G1	THR	346	47.870	-4.523	64.301	1.00 19.38	В
	MOTA	5074		THR	346	46.520	-6.467	63.721	1.00 15.93	В
	MOTA	5075	Ċ	THR	346	44.888	-6.075	66.057	1.00 14.75	В
	ATOM	5076	ŏ	THR	346	43.863	-6.320	65.403	1.00 12.97	В
70		5077			347	45.210	-6.741	67.165	1.00 15.11	В
10	MOTA		N	LEU						В
	ATOM	5078	CA	LEU	347	44.371	-7.819	67.693	1.00 14.94	
	MOTA	5079	CB	LEU	347	45.080	-8.601	68.797	1.00 13.17	В
	MOTA	5080	CG	LEU	347	46.253	-9.465	68.342	1.00 12.75	В

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	MOTA	5081	CDI	LEU	347	46 845	-10.156	69.559	1.00 9.82	В
	ATOM	5082		LEU	347	45.781	-10.459	67.281	1.00 10.19	В
	ATOM	5083		LEU	347	43.074	-7.289	68.277	1.00 14.55	В
			C						1.00 14.55	B
5	ATOM	5084	0	LEU	347	42.039	-7.935	68.196		
,	ATOM	5085	N	SER	348	43.127	-6.107	68.872	1.00 14.94	В
	MOTA	5086	CA	SER	348	41.917	-5.534	69.425	1.00 12.88	В
	ATOM	5087	CB	SER	348	42.236	-4.288	70.204	1.00 11.62	В
	MOTA	5088	0G	SER	348	42.841	-4.656	71.416	1.00 18.29	В
	MOTA	5089	С	SER	348	40.974	-5.180	68.303	1.00 12.87	В
10	MOTA	5090	0	SER	348	39.809	-5.505	68.355	1.00 12.88	В
	MOTA	5091	N	THR	349	41.494	-4.518	67.281	1.00 12.34	В
	ATOM	5092	CA	THR	349	40.672	-4.121	66.151	1.00 14.07	В
	ATOM	5093	CB	THR	349	41.515	-3.400	65.081	1.00 14.87	В
				THR			-2.096			
15	MOTA	5094			349	41.887		65.535	1.00 17.94	В
13	MOTA	5095	CG2		349	40.738	-3.238	63.828	1.00 15.48	В
	MOTA	5096	С.	THR	349	39.992	-5.321	65.493	1.00 16.16	В
	MOTA	5097	0	THR	349	38.770	-5.325	65.282	1.00 15.82	В
	MOTA	5098	N	LEU	350	40.777	-6.339	65.157	1.00 15.00	В
	MOTA	5099	CA	LEU	350	40.226	-7.518	64.508	1.00 15.08	В
20	MOTA	5100	CB	LEU	350	41.352	-8.496	64.206	1.00 14.08	В
	MOTA	5101	CG	LEU	350	41.963	-8.503	62.812	1.00 10.95	В
	MOTA	5102		LEU	350	42.004	-7.143	62.214	1.00 10.81	В
	MOTA	5103		LEU	350	43.347	-9.038	62.947	1.00 11.99	В.
	MOTA	5104	c	LEU	350	39.162	-8.172	65.367	1.00 16.48	В
25	ATOM	5105	ò	LEU	350	38.132	-8.595	64.876	1.00 17.28	В
23									1.00 17.28	В
	MOTA	5106	N	GLU	351	39.443	-8.254	66.658		
	MOTA	5107	CA	GLU	351	38.514	-8.B42	67.609	1.00 19.87	В
	MOTA	5108	CB	GLU	351	39:144	-8.846	69.003	1.00 21.84	В
20	MOTA	5109	CG	GLU	351	38.494	-9.791	69.965	1.00 26.42	8
30	ATOM	5110	CD	GLU	351	38.420	-11.196	69.403	1.00 30.21	В
	MOTA	5111	OE1	GLU	351	39.481	-11.771	69.051	1.00 29.53	В
	MOTA	5112	OE2	GLU	351	. 37.289	-11.724	69.309	1.00 32.89	В
	MOTA	5113.	С	GLU	351	37.217	-8.024	67.646	1.00 19.18	В
	MOTA	5114	0	GLU	351	36.126	-8.569	67.714	1.00 19.57	В
35	MOTA	.5115	N	TYR	352	37.368	-6.703	67.603	1.00 18.87	В
	ATOM	5116	CA	TYR	352	36.258	-5.756	67.646	1.00 17.30	В
	MOTA	5117	CB	TYR	352	36.816	-4.348	67.891	1.00 14.25	В
		5118		TYR			-3.239	68.039	1.00 11.72	В
	ATOM		CC		352	35.794				
40	MOTA	5119		TYR	352	35.105	-2.729	66.933	1.00 11.26	В
40	ATOM	5120	CE1		352	34.220	-1.649	67.067	1.00 11.17	В
	ATOM	5121		TYR	352	35.570	-2.654	69.282	1.00 10.15	В
	MOTA	5122	CE2	TYR	352	34.699	-1.584	69.433	1.00 9.37	В
	MOTA	5123	CZ	TYR	352	34.024	-1.078	68.322	1.00 11.62	В
4.5	MOTA	5124	OH	TYR	352	33.175	0.010	68.445	1.00 14.22	8
45	MOTA	5125	C	TYR	352	35.442	-5.814	66.362	1.00 18.80	В
	MOTA	5126	0	TYR	352	34.217	-5.852	66.407	1.00 19.93	В
	ATOM	5127	N	ALA	353	36.115	-5.822	65.216	1.00 18.33	В
	MOTA	5128	CA	ALA	353	35.406	-5.891	63.951	1.00 17.31	В
	ATOM	5129	СВ	ALA	353	36.359	-5.698	62.821	1.00 16.39	В
50	MOTA	5130	c	ALA	353	34.680	-7.221	63.785	1.00 18.36	В
	ATOM	5131	ŏ	ALA	353	33.542	-7.249	63.365	1.00 18.10	В
	MOTA	5132	N	HIS	354	35.354	-8.319	64.119	1.00 19.39	В
						34.779	-9.661		1.00 20.34	В
	MOTA	5133	CA	HIS	354			63.994		
55	ATOM	5134	CB	HIS	354	35.761	-10.712	64.509	1.00 22.75	В
22	MOTA	5135	CC	HIS	354	35.302	-12.121	64.294	1.00 25.34	В
	MOTA	5136		HIS	354	34.797	-13.031	65.156	1.00 25.57	В
	MOTA	5137	ND1	HIS	354	35.311	-12.725	63.053	1.00 25.77	В
	MOTA	5138		HIS	354	34.831	-13.948	63.164	1.00 26.03	В
	ATOM	5139	NE2	HIS	354	34.511	-14.162	64.427	1.00 26.67	В
60	ATOM	5140	С	HIS	354	33.486	-9.811	64.796	1.00 20.23	В
	MOTA	5141	0	HIS	354		-10.417	64.352	1.00 18.53	В
	ATOM	5142	N	ARG	355	33.505	-9.255	65.995	1.00 20.24	В
	ATOM	5143	CA	ARG	355	32.370	-9.285	66.891	1.00 20.90	В
	ATOM									
65		5144	CB	ARG	355	32.823	-8.721	68.239	1.00 20.70	В
UJ	ATOM	5145	CC	ARG	355	31.789	-8.672	69.339	1.00 21.77	В
	ATOM	5146	CD	ARG	355	32.433	-8.121	70.598	1.00 22.76	В
	MOTA	5147	NE	ARG	355	31.461	-7.943	71.673	1.00 27.66	В
	ATOM	5148	CZ	ARG	355	30.820	-8.942	72.281	1.00 31.26	В
~ 0	MOTA	5149		ARG	355	31.042	-10.206	71.921	1.00 31.17	В
70	ATOM	5150	NH2	ARG	355	29.965	-8.679	73.262	1.00 31.12	В
	MOTA	5151	С	ARG	355	31.177	-8.513	66.305	1.00 21.80	В
	MOTA	5152	ō	ARG	355	30.040	-8.932	66.453	1.00 23.53	В
	ATOM	5153	N	ALA	356	31.442	-7.394	65.634	1.00 21.31	В

	ATOM	5154	CA	ALA	356	30.375	-6.586	65.049	1.00 20.41	В
	ATOM	5155	CB	ALA	356	30.924	-5.282	64.583	1.00 20.58	В
		5156	c	ALA	356	29.618	-7.256	63.902	1.00 20.99	В
	MOTA									
~	MOTA	5157	0	ala	356	28.531	-6.796	63.543	1.00 19.69	В
5	MOTA	5158	N	LYS	357	30.195	-8.328	63.340	1.00 22.58	В.
	ATOM	5159	CA	LYS	357	29.590	-9.081	62.225	1.00 22.82	В
	ATOM	5160	CB	LYS	357		-10.371	61.911	1.00 23.14	В
	MOTA	5161	CG	LYS	357		-10.194	61.443	1.00 25.46	В
	ATOM	5162	CD	LYS	357	31.897	-10.597	59.983	1.00 27.85	В
10	MOTA	5163	CE	LYS	357	31.660	-12.104	59.763	1.00 27.26	В
	ATOM	5164	NZ	LYS	357	32.648	-12.966	60.485	1.00 27.32	· в
				LYS	357			62.594		В
	ATOM	5165	C			28.198	-9.551		1.00 23.74	
	MOTA	5166	0	LYS	357	27.315	-9.635	61.755	1.00 22.43	В
	ATOM	5167	N	ASN	358	28.016	-9.845	63.876	1.00 25.58	В
15	ATOM	5168	CA	ASN	358	26.730	-10.306	64.388	1.00 28.23	В
	ATOM	5169	CB	ASN	358		-10.928	65.766	1.00 28.39	В
								65.742		
	MOTA	5170	CG	ASN	358		-12.105		1.00 29.97	В
	ATOM	5171	OD1	ASN	358	28.203	-12.649	66.778	1.00 31.69	В
	MOTA	5172	ND2	ASN	358	28.267	-12.506	64.551	1.00 29.57	В
20	ATOM	5173	С	ASN	358	25.606	-9.270	64.476	1.00 30.00	В
	ATOM	5174	ō	ASN	358	24.487	-9.619	64.845	1.00 30.93	В
	MOTA	5175	N	ILE	359	25.892	-8.011	64.152	1.00 31.11	В
	MOTA	5176	CA	ILE	359	24.855	-6.986	64.176	1.00 32.09	В
	ATOM	5177	CB	ILE	359	25.465	-5.604	64.142	1.00 31.91	• в
25	ATOM	5178	CG2	ILE	359	24.367	-4.569	64.136	1.00 30.39	В
	MOTA	5179		ILE	359	26.375	-5.433	65.361	1.00 32.12	. В
	MOTA	5180		ILE	359	27.169	-4.134	65.382	1.00 34.29	В
	ATOM	5181	С	ILE	359	23.903	-7.152	62.984	1.00 33.89	В
	ATOM	5182	0	ILE	359	24.326	-7.355	61.843	1.00 32.83	В
30	MOTA	5183	N	LEU	360	22.605	-7.080	63.256	1.00 36.27	В
-									1.00 39.23	В
	MOTA	5184	CA	LEU	360	21.597	-7.249	62.211		
	MOTA	5185	CB	LEU	360	20.630	-8.381	62.583	1.00 42.29	В
	MOTA	5186	CG	LEU	360	19.497	-8.742	61.609	1.00 44.94	B
	MOTA	5187	CD1	LEU	360	20.073	-9.122	60.240	1.00 44.70	В
35	ATOM	5188		LEU	360	18.676	-9.901	62.188	1.00 45,24	В
23	ATOM						-5.970	62.028	1.00 39.70	В
		5189	С	LEU	360	20.800				
	MOTA	5190	0	LEU	360	20.286	-5.429	62.994	1.00 39.55	В
	ATOM	5191	N	ASN	361	20.710	-5.509	60.777	1.00 40.33	В
	-ATOM	5192	CA	ASN	361	19.989	-4.286	60.413	1.00 39.80	В
40	ATOM	5193	СВ	ASN	361	20.865	-3.358	59.573	1.00 40.62	В
. •				ASN					1.00 41.69	В
	ATOM	5194	CG		361	22.050	-2.798	60.350		
	MOTA	5195		ASN	361	22.893	-2.087	59.792	1.00 41.21	В
	MOTA	5196	ND2	ASN	361	22.119	-3.109	61.633	1.00 41.78	В
	MOTA	5197	С	ASN	361	18.748	-4.575	59.575	1.00 40.40	В
45	MOTA	5198	0	ASN	361	18.630	-5.637	58.974	1.00 41.33	В
	ATOM	5199	N				-3.604	59.535	1.00 40.64	В
				LYS	362	17.838				
	MOTA	5200	CA	LY\$	362	16.572	-3.687	58.795	1.00 40.39	В
	MOTA	5201	CB	LYS	362	16.811	-3.781	57.283	1.00 38.42	В
	MOTA	5202	CG	LYS	362	17.283	-2.481	56.664	1.00 37.04	В
50	MOTA	5203	CD	LYS	362	17.312	-2.553	55.151	1.00 35.58	В
	ATOM	5204	CE	LYS	362	15.915	-2.479	54.570	1.00 35.06	B
	MOTA	5205	NZ	LYS	362	15.248	-1.182	54.828	1.00 33.80	В
	MOTA	· 5206	С	LYS	362	15.654	-4.833	59.222	1.00 40.02	В
	ATOM	5207	0	LYS	362	15.341	-5.705	58.378	1.00 41.01	В
55	ATOM	5208	OXT	LYS	362	15.244	-4.848	60.404	1.00 38.46	В
	ATOM	5209	MG	MG	2602	43.447	10.556	59.883	1.00 1.46	
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	MOTA	5239	01B	ADP	2600	45.185	7.724	61.540	1.00 6.06	ADP
	MOTA	5240	02B	ADP	2600	44.098	5.627	60.595	1.00 9.47	· ADP
60	MOTA	5241	03B	ADP	2600	43.494	7.932	59.799	1.00 9.32	ADP
- •	ATOM					45 655				
		5242		ADP	2600	45.933	7.683	57.885	1.00 15.76	ADP
	MOTA	5243		ADP	2600	44.910	7.319	56.926	1.00 19.46	ADP
	MOTA	5244	02A	ADP	2600	45.886	9.129	58.130	1.00 18.59	ADP
	MOTA	5245	03A	ADP	2600	45.669	6.908	59.185	1.00 14.04	ADP
65	ATOM	5246		ADP	2600	47.412	7.404	57.328	1.00 19.34	ADP
	MOTA	5247		ADP.	2600	48.489	6.585	57.824	1.00 22.53	ADP
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70	ATOM	5251		ADP	2600	50.670	8.755	55.611	1.00 26.52	ADP
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	MOTA	5252		ADP	2600	49.154	7.243	54.456	1.00 25.11	ADP
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                                            44.551
                                                     17.713
                                                              49.505
                                                                        1.00 25.90
                                                                                          4-2A
       ATOM
               5306
                      C24 4-2A
                                            44.289
                                                     16.370
                                                              49.394
                                                                        1.00 26.52
                                                                                          4-2A
       MOTA
                                                                       1.00 26.97
1.00 26.51
1.00 27.62
       ATOM
               5307
                      N26-4-2A
                                            40.109
                                                     13.877
                                                              50.027
                                                                                          4-2A
                                                              50.732
51.093
                                            38.991
39.211
                                                     14.325
15.740
                                                                                          4-2A
              5308
5309
                      C27 4-2A
                                   1
       MOTA
                      C28 4-2A
                                                                                           4-2A
       ATOM
30
                                            37.745
                                                     13.725
                                                              51.140
                                                                        1.00 26.04
                                                                                          4-2A
       HOTA
               5310
                      C29 4-2A
                                                                       1.00 26.80
1.00 27.44
       MOTA
               5311
                      C30 4-2A
                                            36.783
                                                     14.431
                                                              51.909
                                                                                          4-2A
                                                                                          4-2A
                                            37.035
                                                     15.782
                                                              52.312
       MOTA
               5312
                      C31 4-2A
                                    1
                                            38.217
                                                     16.439
                                                              51.892
                                                                        1.00 27.46
                                                                                           4-2A
       ATOM
               5313
                      C32 4-2A
                                    1
       MOTA
               5314
                      037 4-2A
                                    1
                                            43.236
                                                     19.647
                                                              49.683
                                                                        1.00 24.48
                                                                                           4-2A
35
               5315
                      038 4-2A
                                            45.096
                                                     15.436
                                                              49.375
                                                                        1.00 27.32
                                                                                          4-2A
       MOTA
       ATOM
               5316
                    C39 4-2A
                                            45.831 18.372 49.744
                                                                       1.00 25.80
                                                                                          4-2A
       END
```

TABLE 5

807

MOTA

OE2 GLU

118

```
40
        REMARK 1 kin_16dpb molecule B

REMARK r= 0.2114 free_r= 0.2639

REMARK rmsd bonds= 0.006712 rmsd angles= 1.32262

REMARK B rmsd for bonded mainchain atoms= 2.570 target= 1.5

REMARK B rmsd for angle mainchain atoms= 2.729 target= 2.0

REMARK B rmsd for angle sidechain atoms= 3.936 target= 2.5

REMARK sg= P2(1)2(1)2(1) a= 69.48 b= 79.54 c= 158.98 alpha= 90. beta= 90. gamma= 90.
45
         REMARK reflection file= k2a.cv
50
        REMARK B-correction resolution: 6.0 - 2.5
         REMARK FILENAME= kin_16dpb.pdb*
ATOM 788 N GLU 116
ATOM 789 CA GLU 116
ATOM 789 CA GLU 116
                                                     39.151
                                                                  9.227 52.663 1.00
                                                                                               8.87
                                                      39.430 10.450
                                                                            51.915
                                                                                       1.00
                                                                                                8.17
                                                      39.921
         MOTA
                   790 CB GLU
                                        116
                                                                11.534
                                                                           52.868
                                                                                      1.00 8.92
                                                                                                             В
                                                                                      1.00 12.15
55
                   791 CG GLU
792 CD GLU
                                                     38.920
39.349
                                                                            53.939
         MOTA
                                        116
                                                                11.894
                                                                13.091
                                                                            54.738
                                                                                       1.00 15.35
                                        116
         ATOM
                    793 OE1 GLU
                                         116
                                                      40.362
                                                                13.717
         MOTA
                                                                            54.354
                                                                                       1.00 17.99
                    794 OE2 GLU
                                         116
                                                      38.678
                                                                13.410
                                                                            55.737
                                                                                       1.00 15.94
         MOTA
                   795 C GLU
796 O GLU
797 N GLY
798 CA GLY
         MOTA
                                        116
                                                      40.426
                                                                10.321
                                                                            50.784
                                                                                       1.00 8.20
60
                                                                10.736
9.744
                                                                           49.657
51.097
                                                                                       1.00
                                                                                               4.89
         MOTA
                                        116
                                                      40.163
                                                     41.577
42.619
                                                                                       1.00
                                                                                               9.09
         MOTA
                                         117
                                                                 9.608
                                         117
                                                                            50.104
                                                                                       1.00 10.26
         ATON
                    799 C GLY
                                                      43.531
                                                                10.819
                                                                            50.183
                                                                                       1.00 11.18
         ATOM
                                         117
                                                                           50.951
49.389
49.386
                   800 O
                                GLY
                                         117
                                                      43.289
                                                                 11.751
                                                                                       1.00 10.98
         MOTA
65
                                                                                       1.00 13.18
                                                      44.590
45.531
                                                                10.813
         ATOM
                   801 N
                                GLU
                                         118
                                                                                                             В
                                                                 11.922
                                                                                       1.00 14.36
                                         118
         MOTA
                   802 CA GLU
         ATOM
                   803
                          CB GLU
                                         118
                                                      46.849
                                                                 11.498
                                                                            50.043
                                                                                       1.00 15.18
                                         118
                                                                 10.756
                                                                            51.363
                                                                                       1.00 21.23
        ATOM
                    804 CG
                               GLU
                                                      46.685
                                                                                       1.00 24.46
         MOTA
                   805
                          CD GLU
                                         118
                                                      48.014
                                                                10.310
                                                                            51.970
                                                                                                             B
70
        ATOM
                   806
                          OEL GLU
                                         118
                                                      48.894
                                                                  9.845
                                                                            51.215
                                                                                                             В
```

48.177

10.413

53.205

1.00 26.10

	ATOM	808	С	GLU	118	45.770	12.281	47.933	1.00 13.80	В
	ATOM	809	ŏ	GLU	118	45.126	11.734	47.041	1.00 14.44	B
	ATOM	810	N	ARG	119	46.689	13.201	47.685	1.00 13.24	В
	MOTA	811	CA	ARG	119	46.984	13.568	46.315	1.00 14.66	В
5	MOTA	812	CB	ARG	119	47.120	15.088	46.167	1.00 12.36	B
	MOTA	813	CG	ARG	119	45.879	15.905	46.518	1.00 11.10	B B
	ATOM	814	CD	ARG	119	44.628	15.371	45.842	1.00 12.06	B
	ATOM	815	NE	ARG	119	44.829	15.087	44.422	1.00 14.81	В
10	ATOM	816	CZ	ARG	119	44.750	15.992	43.451 43.742	1.00 13.37	В
10	MOTA	817	NH1		119	44.464 44.964	17.257 15.632	42.189	1.00 11.75	В
	MOTA	818	NH2		119 119	48.288	12.911	45.889	1.00 16.73	В
	MOTA	819 820	С О	ARG ARG	119	49.253	12.857	46.662	1.00 17.59	В
	MOTA	879	N	TRP	127	42.371	15.847	40.233	1.00 18.06	В
15	ATOM ATOM	880	CA	TRP	127	41.717	15.171	41.335	1.00 16.78	В
13	ATOM	881	CB	TRP	127	40.912	16.167	42.178	1.00 14.46	В
	ATOM	882	CG	TRP	127	39.646	16.618	41.539	1.00 10.93	В
	ATOM	883		TRP	127	38.365	15.996	41.664	1.00 8.71	В
	MOTA	884	CE2	TRP	127	37.452	16.770	40.915	1.00 9.40	В
20	MOTA	885	CE3	TRP	127	37.901	14.857	42.334	1.00 7.23	B B
	MOTA	886	CD1	TRP	127	39.474	17.709	40.738	1.00 10.58	В
	MOTA	887	NE1		127	38.153	17.810	40.361	1.00 8.88 1.00 9.55	В.
	ATOM	888		TRP	127	36.095	16.446	40.820 42.242	1.00 9.73	В
25	MOTA	889		TRP	127	36.545	14.526 15.324	41.488	1.00 11.69	B
25	MOTA	890		TRP	127	35.659 40.828	14.002	40.941	1.00 17.94	В
	MOTA	891	C	TRP TRP	127 127	40.817	12.978	41.621	1.00 18.94	В
	MOTA	892 911	И О	ASP	130	43.130	10.872	40.183	1.00 18.67	В
	MOTA MOTA	912	CA	ASP	130	44.174	10.489	41.121	1.00 17.72	В
30	ATOM	913	CB	ASP	130	44.298	11.534	42.229	1.00 15.27	В
-	MOTA	914	CG	ASP	130	45.675	11.545	42.859	1.00 16.56	В
	MOTA	915		ASP	130	46.157	10.473	43.285	1.00 15.04	В
	ATOM	916	OD2	ASP	130	46.277	12.634	42.930	1.00 16.73	В
	MOTA	917	C	ASP	130	43.921	9.115	41.733	1.00 16.61	В
35	MOTA	- 918	0	ASP	130	42.931	8.905	42.430	1.00 19.40	B B
	MOTA	926	N	LEU	132	45.069	7.791	44.240 45.703	1.00 15.09	В
•	ATOM	927	CA	LEU	132	45.118	7.772 8.487	46.227	1.00 10.29	B
	MOTA	928	CB	LEU	132	46.379 47.765	7.870	45.930	1.00 14.23	В
40	MOTA	929	CG	LEU	132 132	48.877	8.709	46.609	1.00 8.52	В
40	MOTA	930 931		LEU	132	47.829	6.414	46.429	1.00 11.00	В
	MOTA MOTA	932	C	LEU	132	43.858	8.395	46.310	1.00 12.82	В
	MOTA	933	õ	LEU	132	43.719	8.473	47.534	1.00 11.90	В
	MOTA	934	N	ALA	133	42.936	8.833	45.457	1.00 12.47	В
45	MOTA	935	CA	ALA	133	41.681	9.414	45.936	1.00 12.78	В
	MOTA	936	CB	ALA	133	40.826	9.884	44.755	1.00 11.66	В
	MOTA	937	С	ALA	133	40.928	8.356	46.742	1.00 13.76	B B
	MOTA	938	0	ALA	133	40.991	7.163	46.431	1.00 13.92	В
50	MOTA	939	N	GLY	134	40.217	8.798 7.870	47.776 48.619	1.00 13.15	В
50	MOTA	940	CX	GLY	134	39.483 38.016	7.752	48.262	1.00 14.05	В
	MOTA	941 942	С 0	GLY	134 134	37.574	8.262	47.228	1.00 12-84	В
	MOTA MOTA	951	N	ILE	136	35.223	9.141	49.530	1.00 10.60	В
	ATOM	952	CA	ILE	136	34.466	10.377	49.379	1.00 10.62	₿
55	ATOM	953	СВ	ILE	136	34.843	11.386	50.482	1.00 10.47	В
-	ATOM	954	CG2		136	34.175	12.721	50.231	1.00 8.18	В
	ATOM	955		ILE	136	34.382	10.847	51.839	1.00 10.73	. B
	ATOM	956	CD1	ILE	136	34.760	11.746	53.047	1.00 13.23	В
	MOTA	957	С	ILE	136	34.553	11.030	47.995	1.00 11.05	В
60	ATOM	958	0	ILE	136	33.531	11.296	47.373	1.00 10.67	В
	ATOM	959	N	PRO	137	35.765	. 11.303	47.492	1.00 11.64	В
	MOTA	960	CD	PRO	137	37.100	11.313	48.114	1.00 11.30	В
	ATOM	961	CA	PRO	137	35.793	11.924	46.162 46.031	1.00 10.03	В
65	MOTA	962	CB	PRO	137	37.237 38.002	12.410 11.469	46.031	1.00 10.03	В
65	ATOM	963	CG	PRO	137	35.369	10.997	45.019	1.00 11.03	В
	MOTA	964	C	PRO	137 137	34.867	11.455	43.989	1.00 11.71	В
	MOTA	965	0 N	PRO LEU	160	29.446	18.027	56.397	1.00 13.49	В
	MOTA MOTA	1145 1146	N CA	LEU	160	30.595	17.478	57.077	1.00 13.18	
70	MOTA	1147	CB	LEU	160	31.883	18.025		1.00 14.21	В
	MOTA	1148	ČG	LEU	160	33.175	17.477	57.068		
	ATOM	1149		LEU	160	33.056	15.961	57.243	1.00 13.33	
	MOTA	1150		LEU	160	34.343	17.846	56.166	1.00 13.39	В

	MOTA	1151	C LE	ບ 160	30.492	17.857	58.543	1.00 13.90	В
	MOTA	1152	O LE	U 160	30.883	18.956	58.947	1.00 11.88	В.
	MOTA	1564	N TY	R 211	35.581	19.271	44.173	1.00 18.55	В
	MOTA	1565	CA TY	R 211	36.924	19.418	44.731	1.00 18.51	В
5	MOTA	1566	CB TY	R 211	37.994	19.405	43.637	1.00 15.05	В
_	ATOM	1567	CG TY		39.385	19.255	44.201	1.00 14.52	В
	MOTA	1568	CD1 TY		39.721	18.153	44.981	1.00 15.06	В
	ATOM	1569	CE1 TY		40.989	18.023	45.540	1.00 14.43	В
	ATOM	1570	CD2 TY		40.359	20.232	43.988	1.00 13.72	В
10	ATOM	1571	CE2 TY		41.629	20.112	44.541	1.00 12.86	В
10		1572	CZ TY		41.937	19.003	45.316	1.00 13.41	В
	MOTA	1573	OH TY		43.192	18.863	45.864	1.00 13.57	В
	MOTA				37.044	20.683	45.575	1.00 19.47	В
	MOTA	1574	C TY					1.00 21.09	В
15	MOTA	1575	0 77		37.567	20.640	46.688	1.00 13.24	В
15	MOTA	1593	N LE		35.512	20.128	48.935		В
	MOTA	1594	CA LE		36.304	19.274	49.805	1.00 13.61	В
	ATOM	1595	CB LE		36.778	18.022	49.055	1.00 11.20	
	MOTA	1596	CG LE		35.695	17.141	48.423	1.00 12.16	В
20	MOTA	1597	CD1 LE		36.340	15.933	47.756	1.00 10.83	В
20	MOTA	1598	CD2 LE		34.703	16.686	49.485	1.00 11.84	В
	MOTA	1599	C LE		37.503	20.063	50.332	1.00 14.64	B
	MOTA	1600	O LE		37.903	19.885	51.476	1.00 16.56	В
	MOTA	1601	N GI	ນ 215	38.065	20.946	49.506	1.00 16.42	В
	MOTA	1602	CA GI	ນ 215	39.216	21.748	49.930	1.00 18.40	В
25	MOTA	1603	CB GI	JU 215	39.764	22.595	48.781	1.00 18.89	. В
	MOTA	1604	CG GI	ປ 215	40.428	21.819	47.673	1.00 21.62	· B
	ATOM	1605	CD -GI	J 215	40.989	22.739	46.598	1.00 25.34	В
	ATOM	1606	OE1 GI		42.227	22.957	46.572	1.00 24.25	В
	MOTA	1607	OE2 GI		40.182	23.256	45.788	1.00 24.35	В
30	MOTA	1608	C GI		38.856	22.676	51.077	1.00 17.37	В
	MOTA	1609	O GI		39.600	22.779	52.053	1.00 17.62	В
	ATOM	1619	N GI		36.574	22.385	53.343	1.00 17.13	. в
	ATOM	1620	CA GI			21.651	54.586	1.00 16.36	В
	MOTA	1621	C GI		37.821	21.367	55.173	1.00 16.18	В
35	MOTA	1622	O GI		38.044	21.542	56.378	1.00 15.76	В
55	ATOM	1623		A 218	38.746	20.934	54.322	1.00 15.35	В
	ATOM	1624	CA AI		40.105	20.629	54.763	1.00 15.51	В
	MOTA				40.923	20.023	53.596	1.00 14.52	B
		1625			40.806	21.849	55.356	1.00 14.85	В
40	ATOM	1626	C AI				56.386	1.00 15.80	В
40 .	MOTA	1627	O AI		41.470	21.745 22.571	58.714	1.00 13.46	В
-	MOTA	1642	N AJ		39.496			1.00 14.10	В
	ATOM	1643		IG 221	39.917	21.498	59.606		В
	MOTA	1644		kG 221	39.866	20.171	58.853	1.00 13.82	В
15	ATOM	1645		kG 221	39.982	18.949	59.723	1.00 18.08	В
45	ATOM	1646		RG 221	39.939	17.690	58.874	1.00 19.00	
	ATOM	1647		kG 221	38.585	17.167	58.725	1.00 18.62	В
	ATOM	1648	CZ A		38.226	16.296	57.788	1.00 20.44	В
	MOTA	1649	NH1 AF		39.122	15.860	56.905	1.00.20.22	В
~ 0	MOTA	1650	NH2 A		36.980	15.B39	57.751	1.00 16.95	В
50	MOTA	1651		RG 221	41.331	21.780	60.137	1.00 14.31	В
	MOTA	1652		RG 221	41.669	21.408	61.271	1.00 14.60	В
	ATOM	1777	N P	IE 239	30.844	12.531	56.963	1.00 10.36	В
	ATOM	1778	CA PI	iE 239	30.590	13.199	55.695	1.00 10.45	В
	ATOM	1779	CB Pi	IE 239	31.785	13.041	54.753	1.00 10.20	В
55	ATOM	1780	CG P	ie 239	31.691	13.879	53.513	1.00 7.76	В
	MOTA	1781	CD1 Pi	IE 239	30.822	13.533	52.479	1.00 7.06	В
	ATOM	1782	CD2 PI	E 239	32.466	15.026	53.386	1.00 6.02	В
	ATOM	1783	CE1 P	E 239	30.729	14.329	51.327	1.00 7.31	В
	ATOM	1784	CE2 PI	E 239	32.384	15.829	52.242	1.00 6.13	В
60	MOTA	1785	CZ P	IE 239	31.516	15.483	51.210	1.00 5.13	В
	MOTA	1786		E 239	29.350	12.555	55.085	1.00 12.53	В
	ATOM	1787		E 239	29.360	11.369	54.734	1.00 12.06	В
	ATOM	2624	MG MG			10.353	59.884	1.00 13.44	
	ATOM	2625		P 2600		7.176	60.125	1.00 9.41	ADP
65	ATOM	2626	Olb A			7.814	61.350	1.00 10.96	ADP
55	ATOM	2627	OZB AL			5.685	60.429	1.00 12.45	ADP
								1.00 12.43	ADP
	ATOM	2628	03B AI			7.969	59.545	1.00 12.25	ADP
	ATOM	2629	PA AI			7.788	57.787		ADP
70	ATOM	2630	Ola Al			7.466	56.774	1.00 14.66	
70	ATOM	2631	OZA AI			9.225	58.059	1.00 14.40	ADP
	ATOM	2632	03A AI			7.002	59.093	1.00 9.50	ADP
	MOTA	2633	05* AI			7.490	57.279	1.00 16.91	ADP
	MOTA	2634	C5* AI	DP 2600	48.603	6.677	57.812	1.00 18.22	ADP

	ATOM	2635	C4*	ADP	2600	49.807	6.826	56.807	1.00 21.00	ADP
	ATOM	2636	04 *	ADP	2600	49.837	5.609	56.073	1.00 23.65	ADP
	ATOM	2637	C3 *	ADP	2600	49.662	7.936	55.733	1.00 20.88	ADP
	HOTA	2638	03*	ADP	2600	50.883	8.668	55.538	1.00 23.91	ADP
5	ATOM	2639	C2*	ADP	2600	49.227	7.250	54.452	1.00 21.72	ADP
	ATOM	2640	02*	ADP	2600	49.726	7.910	53.286	1.00 24.74	ADP
	MOTA	2641	C1 •	ADP	2600	49.720	5.835	54.648	1.00 22.48	ADP
	ATOM	2642	N9	ADP	2600	48.789	4.775	54.145	1.00 22.01	ADP
	MOTA	2643	C8	ADP	2600	47.775	4.231	54.861	1.00 22.26	ADP
10	ATOM	2644	N7	ADP	2600	47.163	3.322	54.140	1.00 24.15	ADP
	ATOM	2645	C5	ADP	2600	47.742	3.257	52.980	1.00 24.22	ADP
	ATOM	2646	C6	ADP	2600	47.552	2.498	51.838	1.00 25.28	ADP
	ATOM	2647	N6	ADP	2600	46.577	1.596	51.801	1.00 26.60	ADP
	ATOM	2648	Nl	ADP	2600	48.372	2.684	50.738	1.00 28.22	ADP
15	ATOM	2649	C2	ADP	2600	49.388	3.599	50.736	1.00 27.91	ADP
	ATOH	2650	N3	ADP	2600	49.583	4.338	51.852	1.00 25.85	ADP
	MOTA	2651	C4	ADP	2600	48.803	4.199	52.972	1.00 23.75	ADP
	ATOM	2879	C1	5-2b	1	40.179	14.530	46.990	1.00 27.45	5-2b
	MOTA	2880	C2	5-2b	1	41.169	13.921	47.825	1.00 31.74	5-2b
20	HOTA	2881	C3	5-2b	1	42.197	13.109	47.246	1.00 26.68	5-2b
	MOTA	2882	C4	5-2b	1	42.197	12.949	45.832	1.00 25.21	5-2b
	ATOM	2883	C5	5-2b	1	41.213	13.549	44.997	1.00 25.57	5-2b
	MOTA	2884	C6	5-2b	1	40.174	14.358	45.564	1.00 26.52	5-2b
	MOTA	2885	C7	5-2b	1	41.159	14.149	49.287	1.00 39.17	5-2b
25	ATOM	2886	NB	5-2b	1	40.043	13.644	50.068	1.00 32.24	5-2b
	MOTA	2887	C9	5-2b	1	39.077	14.446	50.550	1.00 31.10	5-2b
	MOTA	2888		5-2b	1	39.335	15.753	50.627	1.00 35.90	5-2b
	ATOM	2889		5-2b	1	40.586	16.353	50.204	1.00 43.34	5-2b
00	ATOM	2890		5-2b	1	41.575	15.550	49.725	1.00 51.84	5-2b
30	ATOM	2891		5-2b	1	43.103	12.325	45.318	1.00 22.27	5-2b.
	MOTA	2892		5-2b	1	43.049	15.950	49.559	1.00 69.59	5-2b
	MOTA	2893		5-2b	1	43.510	17.255	49.536	1.00102.78	5-2b
	MOTA	2894		5-2b	1	44.900	17.802	49.405	1.00 94.24	5-2b
25:	MOTA	2895		5-2b	1	44.910	19.338	49.209	1.00 96.86	5-2b
35	MOTA	-2896		5-2b	1	40.562	17.864	50.356	1.00 41.39	5-2b
•	MOTA	2897		5-2b	1	43.806	15.026	49.427	1.00 72.75	5-2b
	MOTA	2898	520	5-2b	1	37.588	13.867	51.069	1.00 18.63	5-2b
	END									•

WHAT IS CLAIMED IS:

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1. A crystallized complex of KSP and a ligand thereof, wherein the relative structural coordinates of the amino acid residues of KSP are as set forth in Table 1 ± the root mean square deviation from the conserved backbone atoms of not more than about 2 Å.

- The crystallized complex of Claim 1, wherein the relative structural coordinates of the amino acid residues are as set forth in
 Table 1 ± the root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 0.5 Å.
 - 3. The crystallized complex of Claim 1, wherein said ligand binds said KSP at a ligand binding site comprising the KSP amino acid residues 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F).
- 4. A crystallized complex of KSP and a ligand thereof,
 wherein the relative structural coordinates of the amino acid residues of KSP
 are as set forth in Table 2 ± the root mean square deviation from the
 conserved backbone atoms of said amino acids of not more than about 2 Å.
- 5. The crystallized complex of Claim 4, wherein the relative structural coordinates of the amino acid residues are as set forth in Table 2 ± the root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 0.5 Å.
- 6. The crystallized complex of Claim 4, wherein said ligand binds said KSP at a ligand binding site comprising the KSP amino acid residues 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F).

7. A crystallized complex of KSP and a ligand thereof, wherein the relative structural coordinates of the amino acid residues of KSP are as set forth in Table 3 \pm the root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 2 Å.

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8. The crystallized complex of Claim 7, wherein the relative structural coordinates of the amino acid residues are as set forth in Table 3 ± the root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 0.5 Å.

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- 9. The crystallized complex of Claim 7, wherein said ligand binds said KSP at a ligand binding site comprising the KSP amino acid residues 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F).
- 10. A crystallized complex of KSP and a ligand thereof, wherein the relative structural coordinates of the amino acid residues of KSP are as set forth in Table $4 \pm$ the root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 2 Å.
- 11. The crystallized complex of Claim 10, wherein the relative structural coordinates of the amino acid residues are as set forth in Table $4 \pm$ the root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 0.5 Å.
- 12. The crystallized complex of Claim 10, wherein said ligand binds said KSP at a ligand binding site comprising the KSP amino acid residues 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F).
- 13. A ligand binding site of a KSP protein comprising the relative structural coordinates set forth in Table 5 ± the root mean square

deviation from the backbone atoms of said amino acids is not more than about 2 Å.

- 14. The ligand binding site of a KSP protein according to
 5 Claim 13 comprising the relative structural coordinates set forth in Table 5 ± the root mean square deviation from the backbone atoms of said amino acids is not more than about 0.5 Å.
- Claim 13 comprising the relative structural coordinates of the KSP amino acid residues 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F) as set forth in a table selected from a group consisting of Tables 1, 2, 3 and 4, ± the root mean square deviation from the backbone atoms of said amino acids is not more than about 2 Å.
 - 16. An agent which binds to the ligand binding site of Claim 13, wherein said agent is an inhibitor of KSP function, or a pharmaceutically acceptable salt thereof.

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- 17. A composition comprising: (a) an agent according to Claim 16; and (b) a pharmaceutically acceptable carrier.
- 18. An agent, or a pharmaceutically acceptable salt

 25 thereof, which binds to five or more of the KSP amino acid residues selected from the group consisting of 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F), wherein said agent is an inhibitor of KSP function.

- 19. A method for identifying an agent that interacts with a ligand binding site of human KSP, comprising the steps of:
 - (a) determining a ligand binding site of KSP from a threedimensional model of the KSP binding site as set forth in

Table 5, \pm the root mean square deviation from the backbone atoms of said amino acids of not more than about 2.0 Å; and

(b) performing computer fitting analysis to identify an agent which interacts with said ligand binding site.

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- 20. A method for identifying an agent that interacts with a ligand binding site of human KSP, comprising the steps of:
- determining a ligand binding site of KSP from a three-dimensional model of KSP using the relative structural coordinates of the KSP amino acid residues 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F) as set forth in a Table selected from the group of Tables 1, 2, 3 and 4, ± the root mean square deviation from the backbone atoms of said amino acids of not more than about 2.0 Å; and
 - (b) performing computer fitting analysis to identify an agent which interacts with said ligand binding site.
- 20 21. A method for identifying a potential inhibitor of KSP function, comprising the steps of:
 - (a) obtaining a three-dimensional model of a KSP binding site wherein said model contains the relative structural coordinates of the ligand binding site of KSP from a threedimensional model of the ligand binding site as set forth in Table 5, ± the root mean square deviation from the backbone atoms of said amino acids of not more than about 2.0 Å;
 - (b) employing said three-dimensional model to design or select a potential inhibitor; and
- 30 (c) synthesizing or obtaining said potential inhibitor.
 - 22. The method according to Claim 21 wherein the potential inhibitor is designed *de novo*.
- 35 23. The method of Claim 21, further comprising the steps of:

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- (d) contacting said potential inhibitor with KSP in the presence of a KSP binding molecule, and
- (e) determining the effect the potential inhibitor has on binding between KSP and the KSP binding molecule.

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- 24. A method for identifying a potential inhibitor of KSP function, comprising the steps of:
 - (a) generating a three-dimensional model of KSP using the relative structural coordinates as set forth in a table selected from Tables 1, 2, 3 and 4, ± a root mean square deviation from the backbone atoms of said amino acids of not more than about 2.0 Å;
 - (b) employing said three-dimensional model to design or select a potential inhibitor; and
- 15 (c) synthesizing or obtaining said potential inhibitor.
 - 25. The method according to Claim 24 wherein the potential inhibitor is designed *de novo*.

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- 26. The method of Claim 24, further comprising the steps of:
- (d) contacting said potential inhibitor with KSP in the presence of a KSP binding molecule, and
- (e) determining the effect the potential inhibitor has on binding between KSP and the KSP binding molecule.

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27. The method of Claim 21, further comprising contacting the potential inhibitor with KSP in the presence of a KSP binding molecule, and determining the effect the potential inhibitor has on binding between KSP and the KSP binding molecule.

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28. The method of Claim 21, further comprising contacting the potential inhibitor with KSP in the presence of one or two

KSP substrates selected from ATP and microtubules, and determining the effect the potential inhibitor has on KSP ATPase activity.

- 29. A potential inhibitor identified by the method of
 5 Claim 21, or a pharmaceutically acceptable salt thereof.
 - 30. A method of identifying an inhibitor compound capable of binding to kinesin spindle protein (KSP), said method comprising:
- (a) introducing protein coordinates selected from the protein coordinates

 provided in a table selected from Tables 1, 2, 3 and 4, ± a root mean

 square deviation from the backbone atoms of said amino acids of not

 more than about 2.0 Å, into a suitable computer program so as to

 define a (+)-monastrol ligand binding site conformation, wherein said

 program displays the three- dimensional structure of the (+)-monastrol

 ligand binding site;
 - (b) creating a three dimensional representation of the (+)-monastrol ligand binding site in said computer program;
 - (c) displaying and superimposing a three dimensional representation of a test compound on the three dimensional representation of the
 (+)-monastrol ligand binding site;
 - (d) assessing whether said test compound fits spatially into the(+)-monastrol ligand binding site;

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- (e) preparing said test compound that fits spatially into the (+)-monastrol ligand binding site;
- (f) using said test compound in a biological assay for KSP function; and
 - (g) determining whether said test compound inhibits KSP function in said assay.
- 31. A process for identifying a potential anti-mitotic agent which upon binding to a human KSP inhibits cell proliferation, the process comprising the steps of:

(a) obtaining an X-ray diffraction pattern of a human kinesin spindle protein (KSP) crystal, wherein said KSP has been crystallized in the presence of a mixture of at least two potential ligands;

- (d) determining whether a ligand/KSP complex is formed by comparing the electron density map calculated from the X-ray diffraction pattern of said KSP crystal to the electron density map calculated from an X-ray diffraction pattern set forth in a table selected from Table 1, 2, 3 and 4; and
 - (c) determining whether said ligand from said ligand/KSP complex binds to the ligand binding site of said KSP according to Claim 15, such that upon binding to KSP said ligand inhibits cell proliferation.
- 32. An anti-mitotic agent identified by the process according to Claim 31, or a pharmaceutically acceptable salt thereof.

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33. A composition comprising: (a) an anti-mitotic agent identified according to Claim 32; and (b) a pharmaceutically acceptable carrier.

20 34. A method of identifying a compound that modulates the binding of a ligand to a ligand binding site of a human KSP, said method comprising: modeling test compounds that fit spatially into a KSP ligand binding site using an atomic structural model of a KSP binding site having the relative structural coordinates as set forth in a table selected from the 25 group consisting of Tables 1, 2, 3 and 4 for the KSP amino acid residues 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F), ± the root mean square deviation from the backbone atoms of said amino acids of not more than about 2.0 Å; screening the test compounds in an assay characterized by binding of a ligand to the ligand 30 binding site; and identifying a test compound that modulates binding of said ligand to the KSP at its binding site.

a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecular complex of a compound bound to the ligand binding site of human KSP, said three-dimensional representation comprising the structural coordinates of the KSP as set forth in a table selected from Tables 1-4 or a homologue of said molecular complex, wherein said homologue comprises a binding site that has a root mean square deviation from the backbone atoms of said KSP of not more than about 2.0 Å.

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- 36. A method for identifying an anti-mitotic agent which upon binding to a target human KSP inhibits cell proliferation, the method comprising the steps of:
 - (a) obtaining a crystal of KSP, where said KSP has been crystallized while exposed to a mixture of at least two potential ligands;
 - (b) determining whether a ligand/KSP complex is formed in said crystal; and
- (c) identifying a potential anti-mitotic agent as one that binds to said KSP

 at a ligand binding site having the relative structural coordinates as set

 forth in Table 5 ± the root mean square deviation of not more than

 about 2.0 Å.
- 37. An anti-mitotic agent identified by the method according to Claim 36, or a pharmaceutically acceptable salt thereof.
 - 38. A composition comprising: (a) an anti-mitotic agent according to Claim 37; and (b) a pharmaceutically acceptable carrier.
- 39. A method for determining the three-dimensional structure of a complex of KSP with a ligand thereof, which comprises obtaining X-ray diffraction data for crystals of the complex comprising the

ligand bound to KSP at a ligand binding site; and utilizing said data to define the three-dimensional structure of the complex.

- 40. A method for evaluating the ability of a chemical

 5 entity to associate with a ligand binding site of human KSP or with at least a
 portion of the site or a complex comprising the KSP binding site; said
 method comprising the steps of:
 - (a) employing computational or experimental means to perform a fitting operation between the chemical entity and said ligand binding site of KSP having the relative structural coordinates as set forth in Table 5 ± the root mean square deviation of not more than about 2.0 Å, thereby obtaining data related to said association; and
- (b) analyzing the data obtained in step (a) to determine the characteristics of the association between the chemical entity and said
 15 KSP or complex.
 - 41. A chemical entity identified by the method of Claim 37, wherein the chemical entity is capable of interfering with the *in vivo* or *in vitro* motor activity of KSP, or a pharmaceutically acceptable salt thereof.
 - 42. A composition comprising: (a) a chemical entity identified according to Claim 38; and (b) a pharmaceutically acceptable carrier.
- 25 43. A method for identifying a potential inhibitor of human kinesin spindle protein (KSP), the method comprising the steps of:
 - (a) providing a three-dimensional structure of a ligand-bound KSP as defined by atomic coordinates set forth in a table selected from a group consisting of Tables 1, 2, 3 and $4 \pm$ the root mean square deviation of not more than about 2.0 Å;
 - (b) comparing the three-dimensional coordinates of the ligand when it is bound to KSP as set forth in Table 1, 2, 3 or $4 \pm$ the root mean square deviation of not more than about 2.0 Å to the three-dimensional coordinates of a compound in a database of compound
- 35 structures; and

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(c) selecting from said database at least one compound that is structurally similar to said ligand when it is bound to said KSP, wherein the selected compound is a potential inhibitor of said KSP.

- 5 44. The method of Claim 43, wherein the structural similarity is determined based on the root mean square deviation in the backbone atoms of the kinesin peptide and the kinesin inhibitor.
- 45. A method for identifying a potential inhibitor of a human kinesin spindle protein (KSP), the method comprising the steps of:
 - (a) providing a three-dimensional structure of said KSP as defined by atomic coordinates set forth in a table selected from Tables 1-4 ± the root mean square deviation of not more than about 2.0 Å;
- (b) employing the three-dimensional structures to design or select a potential inhibitor;
 - (c) synthesizing the potential inhibitor; and
 - (d) contacting the potential inhibitor with KSP to determine the ability of the potential inhibitor to arrest mitosis or inhibit cell proliferation.

- 46. A potential inhibitor identified by the method of Claim 45 or a pharmaceutically acceptable salt thereof.
- 47. A composition comprising: (a) the potential inhibitor identified according to Claim 46; and (b) a pharmaceutically acceptable carrier.
- 48. A method of identifying an inhibitor of KSP wherein the inhibitor binds to the ligand binding site according to Claim 13 which comprises determining the shift in the fluorescence of an amino acid residue at position 127 of KSP, wherein said amino acid residue is tryptophan.
 - 49. The method according to Claim 48 which comprises the steps of:

> (a) contacting KSP with the test compound and a nucleotide and measuring the fluorescence of the mixture at the peak emission wavelength for W127 in KSP;

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contacting KSP with a nucleotide and measuring the (b) fluorescence of the mixture at the peak emission wavelength for W127 in KSP; and

comparing the fluorescence of the mixture of KSP, (c) the test compound and the nucleotide with the fluorescence of the mixture of KSP with the nucleotide alone.

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An anti-mitotic agent characterized as:

(a) specifically binding to the target KSP or an analogue thereof at a ligand binding site comprising the relative structural 15 coordinates of the KSP amino acid residues 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F) according to Tables 1, 2, 20 3 or $4 \pm a$ root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 2.0Å; and

which, upon binding to said KSP or an analogue thereof (b) specifically inhibits said KSP or analogs biological activities.

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- A method of causing the alteration of the structural 51. conformation of a KSP protein which comprises exposing the protein to a ligand that binds to the KSP ligand binding site as set forth in Table 5 ± the root mean square deviation from the backbone atoms of said amino acids of not more than about 2.0 Å.
- The method according to Claim 51 wherein the KSP 52. protein is additionally bound to a nucleotide.

53. A method of treating or preventing hyper-proliferative diseases which comprises administering to a mammal a therapeutically effective amount of a compound that binds to the KSP ligand binding site as set forth in Table $5 \pm$ the root mean square deviation from the backbone atoms of said amino acids of not more than about 2.0 Å.

- 54. The method according to Claim 53 which is a method of treating or preventing cancer.
- 10 55. The method according to Claim 54 which is a method of treating cancer.
- 56. An isolated and substantially pure polypeptide or a fragment thereof comprising the amino acid sequence as set forth in SEQ ID NO:1.
- 57. The isolated polypeptide of Claim 56, wherein the polypeptide adopts the conformation of the ligand binding pocket as set forth in Table 5, ± the root mean square deviation of not more than about 2.0

 20 Å.
 - 58. A variant of the isolated polypeptide according to Claim 57 having at least about 80% amino acid sequence identity with the polypeptide of Claim 57, wherein the percentage identity is determined with the algorithm Gap, BASEFIT or FASTA in the Wisconsin Genetics Software Package release 7.0, using default Gap weights.
- 59. An active structural motif designated herein as pharmacophore model, which refers to the three-dimensional orientation of a set of features describing the physical, chemical and/or electronic environment of the active site of the human KSP, said features comprising either a hydrophobic region feature, a hydrogen bond acceptor feature and a hydrogen bond donor feature (pharmacophore model in FIG. 14A) or two hydrophobic region features and a hydrogen bond acceptor feature (pharmacophore model in FIG. 14B).

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60. A method for screening and identifying potential KSP inhibitor compounds by evaluating the fit of the screened compounds to the pharmacophore models of claim 59.

- 5 61. The method of claim 60 wherein evaluating the fit is carried out via the use of a computer and a computer-readable medium.
- A compound, comprising two hydrophobic region features and a hydrogen bond acceptor feature, wherein said features are oriented as illustrated in
 Figure 14B and wherein said compound inhibits the mitotic kinesin KSP;
 or a pharmaceutically acceptable salt thereof.
- A compound, comprising two hydrophobic region features and a hydrogen bond acceptor feature, wherein said features are oriented as illustrated in
 Figure 14B and wherein said compound fits within a ligand binding site of a kinesin spindle protein (KSP) protein, said ligand binding site comprising the relative structural coordinates set forth in Table 5 ± the root mean square deviation from the backbone atoms of said amino acids of not more than about 2 Å;

or a pharmaceutically acceptable salt thereof.

- 64. The compound according to Claim 63 wherein the two hydrophobic region features are independently selected from an aryl, heteroaryl and C₃-C₇-cycloalkyl, optionally substituted.
- 25 65. The compound according to Claim 63 wherein the two hydrophobic region features are independently selected from an optionally substituted phenyl.
- 66. The compound according to Claim 63 wherein the compound 30 has a binding affinity for KSP of about 0.1nM to about 100nM.
 - 67. A compound, comprising one hydrophobic region feature, a hydrogen bond donor feature and a hydrogen bond acceptor feature, wherein said

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features are oriented as illustrated in Figure 14A and wherein said compound inhibits the mitotic kinesin KSP;

or a pharmaceutically acceptable salt thereof.

68. A compound, comprising one hydrophobic region feature, a hydrogen bond donor feature and a hydrogen bond acceptor feature, wherein said features are oriented as illustrated in Figure 14A and wherein said compound fits within a ligand binding site of a kinesin spindle protein (KSP) protein, said ligand binding site comprising the relative structural coordinates set forth in Table 5 ± the root mean square deviation from the backbone atoms of said amino acids of not more than about 2 Å;

or a pharmaceutically acceptable salt thereof.

- 69. The compound according to Claim 68 wherein the hydrophobic region feature is selected from an aryl, heteroaryl and C₃-C₇-cycloalkyl, optionally substituted.
 - 70. The compound according to Claim 68 wherein the hydrophobic region feature is selected from an optionally substituted phenyl.
 - 71. The compound according to Claim 68 wherein the compound has a binding affinity for KSP of about 0.1nM to about 100nM.
- 72. The compound according to Claim 68 wherein the compound does not comprise a 2-thioxo-1,2,3,4-tetrahydopyrimidine moiety, a dihydropyrimidine moiety or a 5,6,11,11a-tetrahydro-1H-imidazo[1',5':1,6]-pyrido[3.4-b]indole-1,3(2H)-dione moiety.
- 73. A compound, comprising three hydrophobic region features and a hydrogen bond acceptor feature, wherein said features are spatially oriented as illustrated in Figure 16 and have the distances in Å between the features as follows

	1	2	3	4
1	-		1	
2	5.1±0.6			
3	8.5±0.7	6.9±0.7	-	
4	3.7±0.5	5.8±0.6	5.7±0.7	-

and wherein said compound inhibits the mitotic kinesin KSP; or a pharmaceutically acceptable salt thereof.

5 74. The compound according to Claim 73 wherein the compound does not comprise a quinazolinone, phenothiazine, thienopyrimidinone, furanopyrimidinone, azolopyrimidinone, thiazolopyrimidine, cycloalkylpyrimidinone or triphenylmethane moiety.

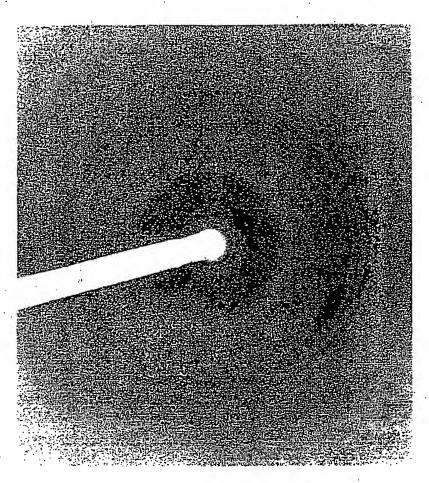


FIG.1

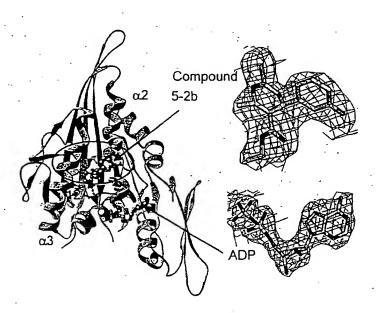


FIG.2

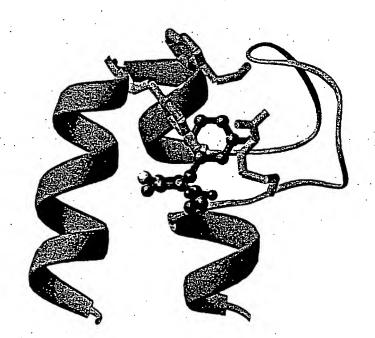


FIG.3

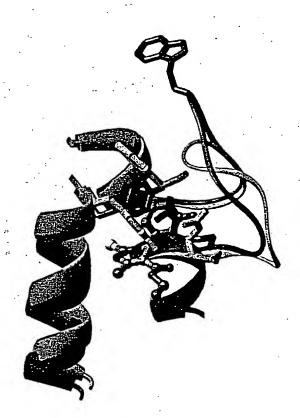


FIG.4

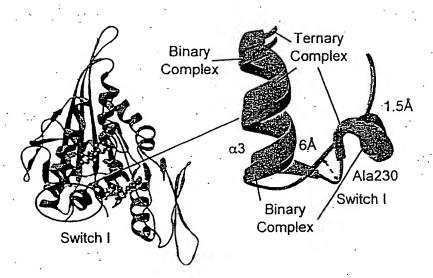


FIG.5

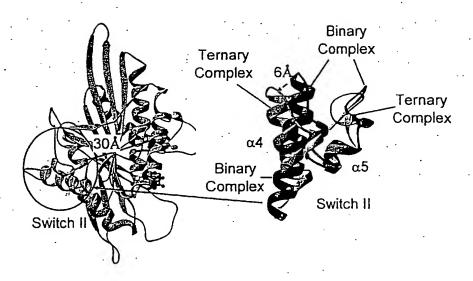


FIG.6

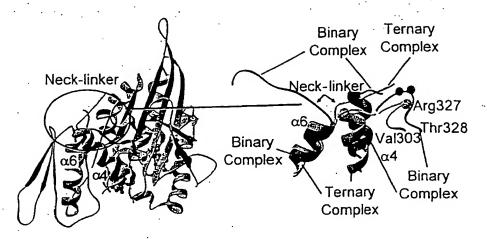


FIG.7

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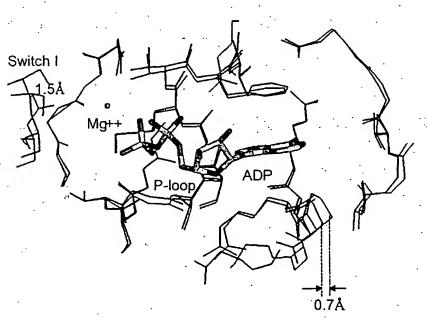


FIG.8

.Seq. ID #1

MASQPNSSAK KKEEKGKNIQ VVVRCRPFNL AERKASAHSI VECDPVRKEV SVRTGGLADK SSRKTYTFDM VFGASTKQID VYRSVVCPIL DEVIMGYNCT IFAYGQTGTG KTFTMEGERS PNEEYTWEED PLAGIIPRTL HQIFEKLTDN GTEFSVKVSL LEIYNEELFD LLNPSSDVSE RLQMFDDPRN KRGVIIKGLE EITVHNKDEV YQILEKGAAK RTTAATLMNA YSSRSHSVFS VTIHMKETTI DGEELVKIGK LNLVDLAGSE NIGRSGAVDK RAREAGNINQ SLLTLGRVIT ALVERTPHVP YRESKLTRIL QDSLGGRTRT SIIATISPAS LNLEETLSTL EYAHRAKNIL NKPEVNQK

FIG.9

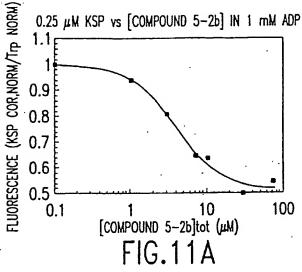
115(M), 116(E), 117(G), 118(E), 119(R);

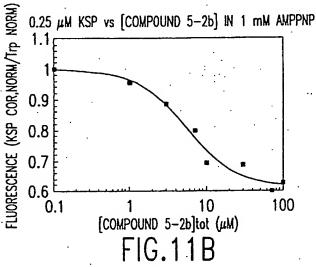
127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P);

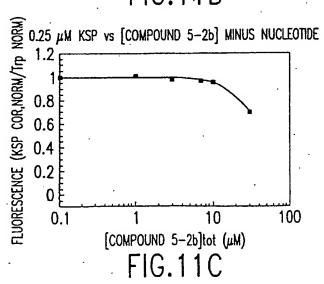
160(L); and

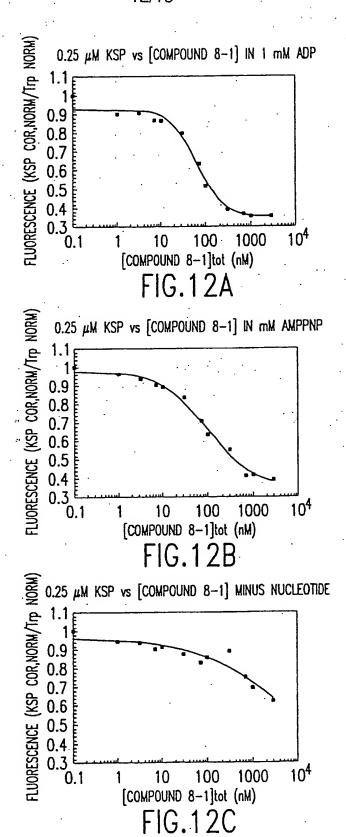
211(Y), 214(L), 215(E), 217(G), 218(A), 221(R), 239(F).

FIG.10

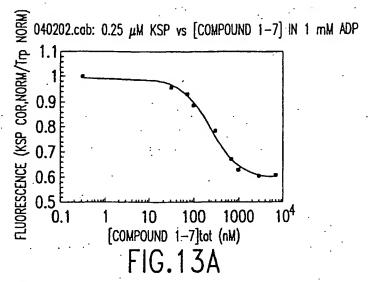


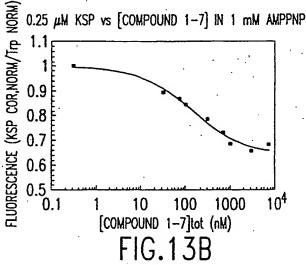


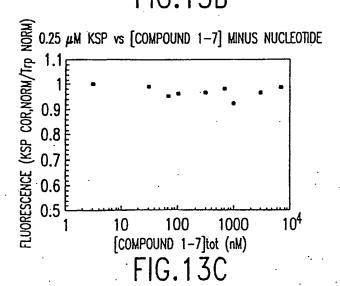












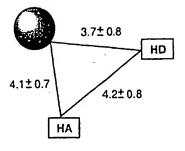


FIG. 14A

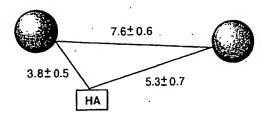


FIG. 14B

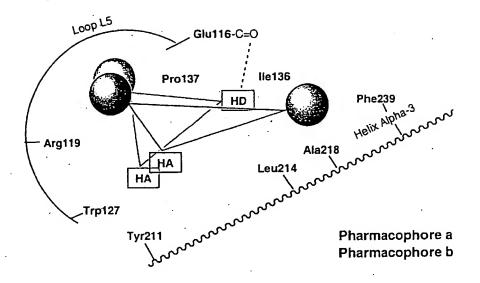


FIG. 15

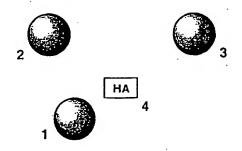


FIG. 16

SEQUENCE LISTING

<110> Merck & Co., Inc.
 Buser-Doepner, Carolyn A.
 Coleman, Paul J.
 Cox, Christopher D.
 Fraley, Mark E.
 Garbaccio, Robert M.
 Hartman, George D.
 Heimbrook, David C.
 Huber, Hans E.
 Kuo, Lawrence C.
 Sardana, Vinod V.
 Torrent, Maricel
 Youwei, Yan

<120> MITOTIC KINESIN BINDING SITE

<130> 21125Y

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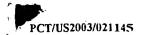
<213> human

<400> 1

Met Ala Ser Gln Pro Asn Ser Ser Ala Lys Lys Glu Glu Lys Gly 1 10 Lys Asn Ile Gln Val Val Val Arg Cys Arg Pro Phe Asn Leu Ala Glu 20 25 30 Arg Lys Ala Ser Ala His Ser Ile Val Glu Cys Asp Pro Val Arg Lys 35 -40 45 Glu Val Ser Val Arg Thr Gly Gly Leu Ala Asp Lys Ser Ser Arg Lys Thr Tyr Thr Phe Asp Met Val Phe Gly Ala Ser Thr Lys Gln Ile Asp Val Tyr Arg Ser Val Val Cys Pro Ile Leu Asp Glu Val Ile Met Gly 85 90 Tyr Asn Cys Thr Ile Phe Ala Tyr Gly Gln Thr Gly Thr Gly Lys Thr 100 105 110 Phe Thr Met Glu Gly Glu Arg Ser Pro Asn Glu Glu Tyr Thr Trp Glu 115 120 125 Glu Asp Pro Leu Ala Gly Ile Ile Pro Arg Thr Leu His Gln Ile Phe 130 135 140 Glu Lys Leu Thr Asp Asn Gly Thr Glu Phe Ser Val Lys Val Ser Leu 150 155 160 Leu Glu Ile Tyr Asn Glu Glu Leu Phe Asp Leu Leu Asn Pro Ser Ser

Asp Val Ser Glu Arg Leu Gln Met Phe Asp Asp Pro Arg Asn Lys Arg

170



	180		185		190
Gly Val Il 19	e Ile Lys Gl 5	y Leu Glu 200	Glu Ile Thr	Val His 2	Asn Lys Asp
Glu Val Ty 210	r Gln Ile Le	Glu Lys 215	Gly Ala Ala	Lys Arg ? 220	Thr Thr Ala
Ala Thr Le 225	u Met Asn Al 23		Ser Arg Ser 235	His Ser V	Val Phe Ser 240
Val Thr Il	e His Met Ly 245	Glu Thr	Thr Ile Asp 250	Gly Glu (Glu Leu Val 255
Lys Ile Gl	y Lys Leu As 260	Leu Val	Asp Leu Ala 265		Glu Asn Ile 270
Gly Arg Se 27	r Gly Ala Va 5	l Asp Lys 280	Arg Ala Arg	Glu Ala (Sly Asn Ile
Asn Gln Se 290	r Leu Leu Th	Leu Gly 295	Arg Val Ile	Thr Ala I	Leu Val Glu
Arg Thr Pro	o His Val Pro 31		Glu Ser Lys 315	Leu Thr A	Arg Ile Leu 320
	325		Arg Thr Ser 330		335
	340		Glu Thr Leu 345	3	350
Ala His Ar		Ile Leu 360	Asn Lys Pro	Glu Val A	Asn Gln Lys